Institute *of* Physics

Newsletter

of

The Computational Physics Group

The first thesis prizes in computational physics

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Comments about the newsletter should be sent to Andrew Horsfield

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Dr Webber receiving his prize at the Grid and Visualization meeting.

Chairman's Remarks - Modelling in physics

Peter Borcherds (chairman)

Some ten to twenty years ago many physics undergraduates had considerable computing skills, learned on home microcomputer such as those made by Acorn and Apple. In that time many computers came with a BASIC interpreter which made it easy for beginners to get experience of programming. With both Acorn and Apple computers it was easy to write programs with dynamical graphics displays, e.g to show central body motion.

Starting from BASIC, it was possible for enthusiasts to learn other languages. Currently most home computers come with software for writing letters and performing other office tasks, but with not very much software which leads to programming skills. For that you generally have to pay real money.

However there are software packages available free which can lead to insight into computing and into computational physics. In July The Computational Physics Group and the Education Group of the IoP held a joint meeting on "Modelling in Physics", aimed mainly at how computers may be used in the teaching of physics in schools. We were shown two excellent pieces of free educational software: West Point Bridge Designer and Modellus, on which there are separate notes.

There is also Python, which many of you may be familiar with. This also is available free. This is a language, with excellent graphics facilities, which make it very easy to write simple programs with a graphical display. The display can be rotated and rescaled by means of mouse movements. Some screenshots are shown (see Jpeg files).

Modellus and Python allow beginners to get some experience of real computing (as in "real programmers use FORTRAN"). Of course members of the Computational Physics Group do not need this experience for themselve, but you may have friends or relations (children?) who might find Python or Modellus of interest.

Further information on: Modelling in physics

Peter Borcherds (Chairman)

Modellus

Modellus is a free package. It is about 10Mb, with an additional pdf file of about 1Mb for a manual. This package is intended for 16+ physics teaching, and allows one to model simple mathematics (graph plotting) and numerical methods (e.g. pendulum) using, say, Euler's method. It also includes a "differentiation" routine, using the common 4th order Runge Kutta method. The package comes with work sheets, which are well written and allow you to get started, so that it is straightforward to design your own material. One problem however: Modellus fills the screen, and so does the work sheet, so you have to switch from one to the other unless you have two computers side by side, or are prepared to print out the worksheet. This is a well-designed package, with interesting features, e.g. if you place a ball on the screen, you can "grab" it with a "hand", and move it about.

West Point Bridge Designer

West Point, the US Military Academy, has produced a program called West Point Bridge Designer (WPBD). This allows one to design and test a bridge. It is excellent, and is supported by a manual which explains the design procedure. There is an accompanying book (learning activity) available either as pdf files (25Mb) or as a a paper version you can buy. The book provides a clear explanation of the design process and should be used if you want to make serious use of WPBD.

The learning activity also includes instructions for building a "real" bridge to your computer aided design, using cardboard manilla folders as your raw material. The model you build is 60 cm long, not the 60 feet or so of the bridge you have designed, using steel.

A not uncommon school science project is for a group of students to build a bridge out of materials like card and drinking straws. Having built such a bridge, it can then be tested by placing ever increasing loads on it until it collapses. However while this method of construction and destructive testing may develop communication skills within the group, it does not teach very much science, nor is it the way real bridges are designed.

WPBD comes in various versions: one version was released for a competition (which has now closed) for American Schools (K12) to mark the bicentennial of West Point (another competition is scheduled for 2002-3). This version and version 4 (which appears very similar, but has different sample bridges and templates) is available from the website http://bridgecontest.usma.edu (Click on "download" for the programs and on "resources" for the supporting book). Each program is about 3MB, and is free!) The aim is to design the cheapest possible bridge of specified length which will carry a specified load (a lorry).

When you have designed your bridge, you test it. However if the design is structurally unstable, the program tells you, explains structural stability, and sends you back to the drawing board. When you have a structurally stable design, you can test it by sending a lorry across the bridge. The motion of the lorry across the bridge is quite dramatic, since deflections of the bridge under load are shown with a 10 times magnification (see figure below). When the test is running the members of the bridge are colour coded to show the state of stress: compression is shown by red, tension by blue. The greater the stress, the brighter the colour. As the lorry crosses the bridge, the stresses change, shown by changing colours. If any member fails, the test stops (with the lorry falling into the river). If the bridge has collapsed under its own weight, the lorry stops safely at the river bank.

The package contains some sample designs which will carry the load, but which can be improved (i.e. have their cost reduced). During the design process the cost is shown on the screen. Templates of various types of bridges are provided. The members of the bridges can be chosen to be hollow tubes or solid bars, and there is a choice of different steels. The size (cross section) of each member can be chosen too. Data on the strength of a member is available in the program: a graph showing how compression strength depends upon the length of the member can be displayed.

After testing your design, you can then modify it: any elements which have failed are shown in bright colours. You can consult a table listing all the members, and the maximum stress (both in compression and in tension) each has experienced. Those very lightly stressed can be made smaller, but that does not necessarily reduce the cost of the bridge: the program penalises you if you have too many different sizes of members.

The program has comprehensive documentation, including a section "What is not realistic about WPBD". This section points out that the testing of the bridge is carried out by a lorry moving from left to right, with unequal loading on its two axles: it is thus possible to design an asymmetrical bridge which could collapse if the lorry were to go the other way! It also points out that aesthetics is another aspect of bridge design which is not included.

The program is essentially two-dimensional, so that, for example, crosswinds are ignored. I look forward to an extended version to include a model of Galloping Gertie (Tacoma, 1940).

This package has been developed by Colonel Stephen Ressler of the Department of Civil and Mechanical Engineering at West Point.

Figure 1: Lorry crossing a bridge

Computation using Spatial Solitons

Allan Boardman (Hon. Group Secretary)

In 1834, a fascinating, accidental, discovery was made by John Scott Russell, on a canal near Edinburgh. He observed that it is possible to generate waves with amplitudes large on scale measured in terms of the canal depth. These special waves did not collapse, as might be expected, but travelled on top of the water surface, as isolated humps. He called them solitary waves. Unfortunately, his report to the British Association stirred few imaginations in the nineteenth century. Yet Russell had seen something quite remarkable. He had witnessed nonlinear events that defeated the normal restoring forces.

The realisation that solitary waves are possible in other areas of physics took until 1965, when the word 'soliton' was coined for them in Los Alamos, to illustrate that solitary waves are rather like particles. From that work has evolved the realisation that solitary light waves are also possible.

The modern work began slowly but quite a lot has happened over the last twenty years. On one level, it has led to the acceptance that large amplitude pulses in optical fibres can be used as compact, indestructible, information bits to provide us with even broader highways for the internet. Another possibility is to use beams of light, rather than a pulse. If the power of a light beam is high enough it will increase the refractive index of the material supporting it, through a phenomenon called the optical Kerr effect. The light will then focus in the high index regions near the beam centre. In other words, the high intensity beam will self-focus and try to stop itself from diffracting. A balanced situation occurs when the two physical effects balance. When this happens a spatial soliton (solitary) wave is born. These solitons are compact and usable in an all-optical chip and it is natural to think of them as having a particle-like behaviour. The solitons can carry information characterised by the envelope enclosing the beam, the widths, the positions of the centres, the group and phase velocities, and their relative phases.

Solitary light waves must propagate in real materials so a collision between two, or more, of them will result in an information exchange. It is possible to use these properties of tiny light beams, dashing about on the optical chip of the future, and still maintain their particle properties. People have talked about all-optical computers for a long time now but in earlier years attention was restricted to copying features of a conventional computer, such as discrete gates. With solitary waves we can dispense with all that and encode data as a bundle of solitary waves, injected at the boundary of a chip. As they collide with each other, information transfer is identified as passing on a fraction of energy, shifting their position a little bit, or some other physical property. Indeed, it is possible to construct a general Turing model for this now gateless computing. This is an absolutely fascinating development for the computational power of the future and represents the latest steps towards finding the Holy Grail of all-optical computing. It also shows just how prescient was John Scott Russell, who did try to tell us that solitary waves were everywhere.

Medics get a dose of physics

From physicsweb.org

Spotting dangerous electrical activity in the heart and refining radiation doses in cancer therapies were among the topics discussed today at a conference on Simulation and Modelling Applied to Medicine. Organized by the Institute of Physics, the forum highlighted the growing role of physics in the high-tech world of medicine.

The beating of the heart is controlled by a wave of electrical activity that starts at the sino-atrial node - the heart's natural pacemaker - and spreads outwards. In a healthy heart each wave has faded away by the time the next wave arrives. But if this does not happen, it can lead to a heart attack. Understanding this process - which is known as ventricular fibrillation - is the key to developing new ways to treat the victims of cardiac arrest.

Richard Clayton of the University of Leeds and co-workers at the University of Auckland in New Zealand have developed a computer simulation that shows the electrical patterns in the heart when these faulty beats occur, as shown in this image. Also shown are the 'filaments' that the unstable 're-entrant' waves rotate around. 'Our detailed biophysical and anatomical model can simulate this activity', says Clayton, "and we can then test different pharmacological and physical treatments that could help the patient'.

In the field of radiotherapy, two teams of scientists have devised models that should make treatments safer and more efficient. Norman Kirkby of the University of Surrey worked with engineers and cell biologists from Addenbrooke's Hospital in Cambridge and Mount Vernon Hospital in Middlesex to simulate the multiplication of cancer cells in brain tumours. The growth of such tumours can be stopped if the DNA in these deviant cells is damaged by doses of radiation.

When cancer cells multiply, they go through a cycle that includes a 'self-checking' stage. If the tumour is irradiated during this period, the cells simply repair the damage and keep growing. But the model devised by Kirkby's team could enable doctors to track the cycle so that they can administer radiation treatments at accurate intervals. This means that the cancer cells will be hit when they are most vulnerable, and damage to healthy tissue will be minimized.

Meanwhile, Frank Verhaegen of the National Physical Laboratory and - working independently - Emiliano Spezi at Velindre Hospital in Cardiff have developed Monte Carlo simulations to calculate optimum radiation doses for individual patients. Existing models for calculating such doses are based on simplified physical models and can overlook the different responses of bone and soft tissue to radiation, which may lead to an inaccurate dose.

The Monte Carlo methods developed by Verhaegen and Spezi predict the paths of every particle as it travels from the accelerator and into the patient. This should allow doctors to account for the exact anatomy of each patient when calculating their radiation dose.

The original article was published on 23 January, and can be found at http://physicsweb.org/article/news/6/1/14

Chairman elected to join IUPAP Commission on Computational Physics

Andrew Horsfield

The International Union of Pure and Applied Physics (www.iupap.org) has honoured Peter Borcherds (our Chairman) by electing him to its Commission on Computational Physics. He will serve a three year term beginning immediately, and ending at the General Assembly in the Fall of 2005. I hope you will join me in congratulating him.

Reports on Meetings

Grid Computing & Computer Visualization

Organised by: Andrew Horsfield, Ian Morrison and Richard Ansorge

The meeting was held on Friday 6 September 2002, at the Rutherford Conference Centre, Institute of Physics, London. The speakers, titles and abstracts of the talks are as follows:

1. **Dr Andrew Parker** from *Cambridge University* spoke about SCIENTIFIC APPLICATIONS ON THE GRID. The UK eScience programme has been set up by the Government with funding for three years. Projects are under way in all Research Councils, and in the Core programme which covers more generic work and projects with joint industrial funding. The Cambridge eScience Centre (CeSC) is one of nine regional centres set up under the Core programme, and it supports a variety of projects in different science areas. The talk will give an overview of the programme, and discuss some examples of CeSC projects illustrating the generic themes of distributed computing, distributed data and collaborative visualization.

2. **Prof Mark Sansom** from *Oxford University* spoke about BIOMOLECULAR SIMULATION AND THE GRID. Over the last twenty

years, X-ray crystallography and NMR spectroscopy has revealed the atomic-level detail of many proteins and nucleic acids. However, the atoms from which biomolecules are made are in a state of constant motion at room temperature, and many such molecules function as nanoscale machines. Experimental structural biology methods provide, at best, only clues as to a clear picture of molecular motion, and without this picture our ability to understand the function of these molecules is severely limited.

In an ideal world all simulation data would be available to all interested parties. However, at present simulation data resides in the 'home' laboratory and is not accessible to other research groups. Using the GRID we have an opportunity to draw together distributed collections of simulation data in disparate formats, whilst maintaining a centrally accessible meta-database. There is a pressing need to integrate simulation data more fully with structural biology and bioinformatics databases. For example, we would like to perform simulations more routinely as new, biologically important structures are solved experimentally, and also to exploit the power of modern simulations to explore homology models of biomedically important proteins based on experimental structures, and to explore the structural dynamics of mutant proteins. By setting up a simulation database, we intend to bring about a more systematic and consistent analysis of simulation results. Also, by enabling meta-analysis of the entire database (or significant subsets) and by integrating this database to structural biology databases, we hope to plan future simulations in a more systematic, wide-ranging and comparative fashion. By combining the latter approach with our demonstrated understanding of the relevance of simulations to the drug development process and the pharmaceutical industry, we will more efficiently exploit the results of simulation studies.

3. **Richard Ansorge** from *Cambridge University* spoke about MEDICAL IMAGING AN INTERDISCIPLINARY ESCIENCE OPPORTUNITY. Medical Imaging is a rapidly developing interdisciplinary field. 3D imaging modalities such as PET and MRI can yield very large data sets, which poses challenges in the areas of image reconstruction, image analysis, and visualization and database management. Parallel computing on local PC clusters or high-end systems is an effective tool for these tasks. Several examples from ongoing projects at Addenbrooke's Hospital Cambridge will be given. These projects include MRI and PET image processing and the West Anglia Cancer Network Telemedicine initiative, which involves case conferences between up to eight regional hospitals. A further emerging prospect is data-mining of NHS records for statistical analysis of populations or better diagnosis of individuals.

4. **Ken Brodlie & Jason Wood** from *University of Leeds* spoke about GRID-BASED COLLABORATIVE COMPUTATIONAL STEERING. The talk will describe how existing dataflow visualization systems can evolve to support the new era of Grid computing. We look in particular at IRIS Explorer, a system developed and distributed by NAG Ltd, and show how it can be extended in two significant ways. First, it can extend to support computational steering, where the scientist uses IRIS Explorer as a desktop visual interface to control the operation of a simulation running remotely on a Grid resource. Second, it can extend to allow a geographically-distributed research team to collaborate both in the steering and visualization of a simulation.

   The talk will be illustrated by a demonstrator application which has been built under the UK e-Science programme. This is an environmental application where the release of a dangerous pollutant is modelled, and its dispersion across terrain is predicted in order to guide evacuation strategies.

   The work is being developed further in an e-Science Core Programme project (jointly with the Universities of Oxford and Oxford Brookes, CLRC/RAL, NAG, IBM and Streamline Computing) to develop visualization middleware.

5. **Nick Avis** from *University of Salford* spoke about ADVANCED PROBLEM SOLVING ENVIRONMENTS: COUPLING HPC AND HUMAN SCALE VISUALIZATION FACILITIES. Problem Solving Environments (PSEs) which couple computational steering

techniques with graphical user interfaces and visualization techniques are presently being researched by a number of groups worldwide. Such system allow the human operator to assess and control numerical codes, checkpoint solutions, and often, to allow the sharing of these resources with remote collaborators.

This presentation will highlight the potential (and problems) of coupling such PSEs to large scale Virtual Environment displays such as CAVEs, immersive workbenches and Reality Rooms. The differences between these new PSEs and standard Virtual Environments will be presented. The experiences of conducting numerous sessions in the CAVE at Salford with both local and distributed collaborators will be summarised and some thoughts on the remaining challenges offered.

This work is conducted in collaboration with High Performance Computing Centre Stuttgart (HLRS) and VirCinity and was in part funded by The British Council (Academic Research Collaboration grant - Project 1178).

6. **Steven Kenny** from *Loughborough University* spoke about MATERIALS MODELLING USING LARGE SCALE MD: USING VISUALISATION TO INTERPRET THE DATA. Modern Molecular Dynamics (MD) simulations quite routinely contain upwards of 1 million atoms in the simulated system. These simulations thus generate huge quantities of data which we need to analyse. The traditional solution to this problem is to calculate averaged properties or statistics which massively reduces the data. This does not, however, allow us to analyse the dynamics of the events that occur in the simulation and thus understand features that are seen both in the experiments and the simulations at an atomistic level.

   I will use some different examples of simulations to illustrate how visualisation can be used as a tool for analysing the dynamics of processes. Firstly I will give examples from the simulation of the nanoindentation process. Here we have successfully reproduced a number of experimental results and used MD to elucidate the important atomistic mechanisms that take place allowing us to explain the features seen experimentally. I will then use further examples from the simulation of friction at an atomistic level and from the deposition of clusters onto surfaces.

During the meeting we also had the prize giving for the first of our annual Computational Physics Thesis Prizes (first prize of £500 and two second prizes of £250). The prize winners are listed below. Only Dr Webber was able to attend the meeting to receive his prize in person.

First	Dr Thomas Winiecki	*Numerical Studies of Superfluids and Superconductors*
Second	Dr J.B.W. Webber	*Characterising Porous Media*
	Dr Paula Sanchez-Friera	*Total Energy Calculations from Self-Energy Models*

Upcoming Computational Physics Group Events

Computational Physics Symposium

This symposium is part of the CMMP meeting of the IoP in Belfast. It will take place on the afternoon of Wednesday, April 9^{th}, 2003. Embedding of quantum calculations in classical calculations will be a theme.

Web page: http://www.iop.org/IOP/Confs/

9th Annual MCNEG Meeting

The 9th annual UK Monte Carlo user group meeting ("MCNEG") will be held at the Lister Institute, Edinburgh, Scotland on 31st March / 1st April 2003.

MCNEG comprises members from the healthcare, university and industrial sectors. The meeting brings together the users of primarily Monte Carlo but also deterministic codes and provides a forum in which new developments and projects can be discussed and ideas shared. Although the greatest focus in the past has been on the EGS4/nrc, BEAM and MCNP codes there is active interest in other codes such as GEANT, ETRAN, ITS, FLUKA, PENELOPE, DANTSYS, etc. The meeting covers a broad range of applications in Monte Carlo and deterministic modelling: from radiotherapy, radiation protection and radiological imaging, to nuclear and space engineering.

This year there will be two invited speakers: Prof Alex Bielajew from the University of Michigan, USA who will discuss recent developments in the EGS5 and DPM/PENELOPE codes; and Prof Michel Terrissol, from Universit Paul Sabatier, France, who will consider Monte Carlo methods for microdosimetry and the modelling of DNA/radiation interactions.

The deadline for submission of abstracts is 7th March, 2003.

Attendance at the meeting is £100 (£75 for students) and includes lunch and refreshments on both days.

Web page: http://www.mcneg.org.uk

Beginner's Guide to Quantum Information

On Friday, September 12, 2003, we will hold a meeting at the Institute of Physics, 76 Portland Place, London, that will be an introduction to the theory of quantum information. This meeting will be aimed at those who are interested in the field but are not practitioners.

Web page: http://groups.iop.org/CP/

Biology and Computing

In November 2003, we will hold a meeting at the Institute of Physics, 76 Portland Place, London, that will be focused on the use of computers in biology.

Web page: http://groups.iop.org/CP/

Computer Assessment in Physics

Details will appear on the web page as they become available.

Web page: http://groups.iop.org/CP/

The 2nd Annual Computational Physics Thesis Prize

The Committee of the Institute of Physics Computational Group has endowed two annual prizes. £500 will be awarded to the author of the PhD thesis that contributes most strongly to the advancement of computational physics. The Committee will select the recipients and its remit will be very broad, in order to capture a broad spectrum of modelling activity.

- The deadline for applications is December 31st, 2002.
- The submission format is a 4 page (A4) abstract.
- The submission address is:
  Professor A D Boardman
  Hon. Sec, IoP Computational Physics Group
  Joule Physics Laboratory
  School of Sciences
  University of Salford,
  Salford, M5 4WT

Applicants must have carried out their thesis work at a University in the United Kingdom or the Republic of Ireland.

Other Upcoming Meetings

Scientific computing and its applications

The Third International Workshop on Scientific computing and its applications will be held in Hong Kong from January 6^{th} to January 9^{th} 2003.

Web page: http://math.cityu.edu.hk/sca03

High-performance scientific computing: modelling, simulation and optimisation of complex processes

An International Conference on High-performance scientific computing: modelling, simulation and optimisation of complex processes will be held in Hanoi, Vietnam, from March 10^{th} to 14^{th} 2003.

Web page: http://www.hcmut.edu.vn/hpsc/HPSCHanoi2003

Large-scale scientific computations

The fourth international conference on large-scale scientific computations will be held in Sozopol, Bulgaria from June 4^{th} to 8^{th}, 2003.

Web page: http://parallel.bas.bg/ scicom03

Scientific computing and differential equations

A conference on scientific computing and differential equations will be held in Trondheim, Norway from June 30^{th} to July 4^{th}, 2003.

Web page: http://www.math.ntnu.no/scicade

Computational techniques and applications

The conference on computational techniques and applications will be held within the format of the international Congress of industrial and applied mathematics in Sydney, Australia from July 7^{th} to 9^{th}, 2003.

Web page: http://www.math.ntnu.no/scicade

UKHEC events

UK High-End Computing has a number of upcoming events of interest to physicists. Check the web page for details.

Web page: http://www.ukhec.ac.uk/events/