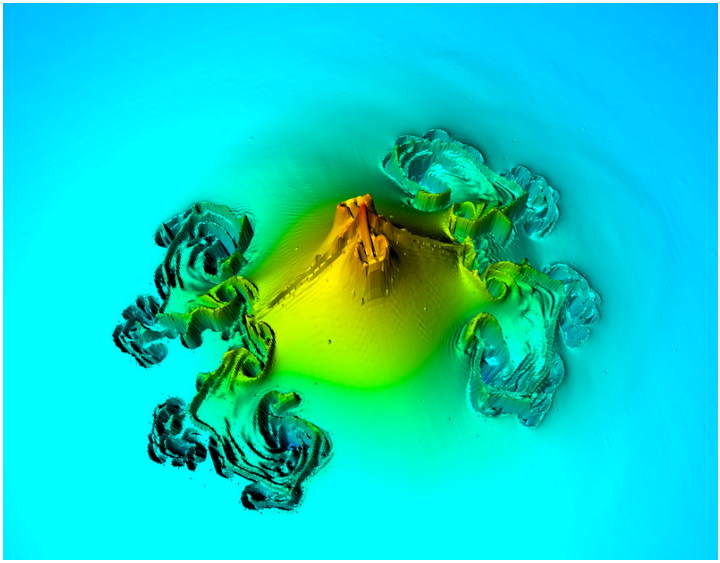
Institute *of* **Physics**

Newsletter

of the

Computational Physics Group



Active Galaxies

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Our web page can be found here: http://groups.iop.org/CP/

Comments about the Newsletter should be sent to Hans Fangohr.

Front cover picture: 2d data of two low-density bubbles buoyantly "ascending" from the centre of gravity of a galaxy cluster in opposite directions. The height of the surface shown corresponds to the density of the gas. (E Pope, G Pavlovksi, C Kaiser and H Fangohr, University of Southampton, 2006)

Newsletter Contents

Heating the Intracluster Medium with Active Galaxies

Edward Pope (University of Leeds), Christian Kaiser, Georgi Pavlovski, Hans Fangohr (University of Southampton)

Introduction

Clusters of galaxies are the largest organised structures in the Universe. These structures can be 10^{25}cm across and typically contain hundreds to thousands of galaxies. The total gravitating masses of galaxy clusters, inferred from galaxy motions, can exceed 10^{48}g, yet roughly only 10% of this is accounted for by visible matter. The remaining constituent is assumed to be dark matter.

The space between the galaxies is not empty, but is filled with tenuous (0.1-0.01 particles per cubic cm), hot gas ($10^7 - 10^8$K) and the mass of this gas is greater than that in visible stars. This gas is referred to as the Intracluster Medium (ICM) and is so hot that it is collisionally ionised and radiates X-rays, primarily due to the thermal bremsstrahlung mechanism.

Since the radiative cooling time of the ICM is much longer than the sound crossing-time the gas forms a quasi-hydrostatic atmosphere. As a result, the gas is necessarily densest near the centre of the cluster's gravitational potential. As a direct consequence, the radiative losses are greatest near the cluster centre, since they are proportional to the square of the density. Then, as the internal energy of the gas is radiated away, the pressure drops and the weight of the overlying gas causes a slow, sub-sonic inflow of material towards the cluster centre. This phenomenon is known as a cooling flow. The radiative losses will also lead to a drop in temperature near the cluster centre. This feature was often considered to be an observable signature of a cooling flow.

The formation of a cooling flow is a positive feedback process: as energy is radiated away, the density of this material increases, further increasing the radiative losses. Unless it is opposed by a heating mechanism, the cooling will eventually become catastrophic and the central temperature of the ICM will become very small, and the central density very large.

Radiative cooling times in the centres of many clusters are significantly less than the age of the Universe. Therefore, we should expect all of the phenomena described above to be observed. In addition, the existence of such a cooling flow would be expected to have deposited large quantities of cold gas near the centre of the cluster. However, observations indicate that the actual mass of cold gas

is less than that predicted by as much as a factor of ten. This discovery, along with evidence from X-ray spectra, suggests that the ICM is heated somehow.

Many possible heat source have been suggested, and almost as many ruled out. Whatever the process is, it must be able to adapt to its surroundings so that it does not overheat, nor underheat, but maintains an approximate steady-state. One logical conclusion to this argument is that the source of heat must be controlled by a negative feedback process, i.e. one that reacts to oppose the action that first caused it. Therefore, a possible heating candidate is energy transport by thermal conduction from the hot outer regions of the cluster, down the temperature gradient, towards the cooler cluster centre. However, this can also be ruled out due to the nature of thermal conduction in cluster: it works for some clusters, but not others. An equally plausible alternative is energy injection from an active galactic nucleus (AGN) located at the centre of the cluster. An AGN is essentially an extremely powerful and compact source of radiation which cannot be attributed to stars, but is accounted for by the accretion of matter onto a supermassive black hole at the centre of a host galaxy. Due to the strong gravity of the black hole, a significant fraction of the rest mass energy of the gas is released. This energy is often observed in the form of extremely powerful, collimated, anti-parallel jets which can propagate at close to the speed of light and sometimes reach a staggering 10^{24}cm in length. Observations indicate that these outflows interact strongly with their environment and so must dissipate a significant fraction of their energy into the surrounding ICM. When applied to galaxy clusters this means that material which has cooled from the ICM is accreted by the central galaxy. The energy released when this material is accreted by the supermassive black hole at the centre of this galaxy is therefore related to the state of the ICM. As energy is fed back to the surroundings, the gas will expand and cooling rate of the ICM will decrease, and therefore the amount of material that reaches the black hole will diminish. Consequently, the power output from the AGN will drop, allowing the ICM cooling rate to increase again. This will increase the amount of material reaching the black hole and the power output from the AGN will increase, and so on. If this is the case, it is possible to concieve that an AGN can control its surroundings.

Another task when investigating the impact of an AGN on its environment is to try and reproduce the correct morphology of the interaction between the jets and their surroundings. For example, certain observational evidence suggests that jets can inflate cavities which seem to be stable to fluid instabilities. Some numerical simulations and analytical work suggest that the only way this can be achieved is by including extra effects such as magnetic fields and viscosity. However, other numerical work suggests that this is not the case, and that these

extra processes are superfluous, although they know doubt play a role at some level.

Method

To study the AGN heating process outlined above it is necessary to employ detailed numerical hydrodynamic simulations. A generic galaxy cluster can be setup using fairly simplistic initial conditions. Firstly, one assumes that the ICM is initially in hydrostatic equilibrium with the dark matter that dominates the gravitational potential of the entire cluster. The functional form of the gravitational potential is usually given by what is commenly referred to as a β-profile model and is spherically symmetric, for simplicity. This is an analytical approximation to the density distribution one expects from a self-gravitating isothermal sphere. A further assumption is that the ICM is initially isothermal, that is the gas temperature is initially independent of radius. This makes the initial density distribution easy to calculate, but is also designed to replicate the true initial conditions of the ICM. The final part of the model is to specify how the radiative losses vary with gas temperature.

Of course, these initial conditions are highly idealised. In reality galaxy clusters grow through successive mergers of galaxy groups and smaller clusters. Such mergers occur relatively frequently and the cluster will rarely be found in a dynamically relaxed state. In principle, it is possible to include these effect by simulating the cosmological growth of structure. However, including so many different physical processes at once makes it difficult to understand to relative importance of each individual process. Specifying relatively simple initial conditions allows us to investigate the properties of a single, or a few, processes.

These simulations were performed using the FLASH hydrodynamics code. FLASH is a Eulerian, adaptive-mesh refinement hydrodynamics code developed and made public by the ASC Centre at the University of Chicago. Using FLASH, the best way to introduce jets to the computational grid is to inject mass, energy and momentum on the boundary. Usually this would be done by specifying an inner boundary near the centre of the grid, however since FLASH does not support polar coordinates this is not possible. The next best option is to cut the initial grid in half by placing an 'inner' boundary across the centre of the grid. Inflow boundary conditions can then be specified near the cluster centre to create the jet, while the boundary conditions along the remainder of the inner boundary were set to reflect. This is in an attempt to mimic the effect of the missing half of the cluster. The external boundary conditions were all set to maintain hydrostatic equilibrium, but allow any disturbances to pass outwards,

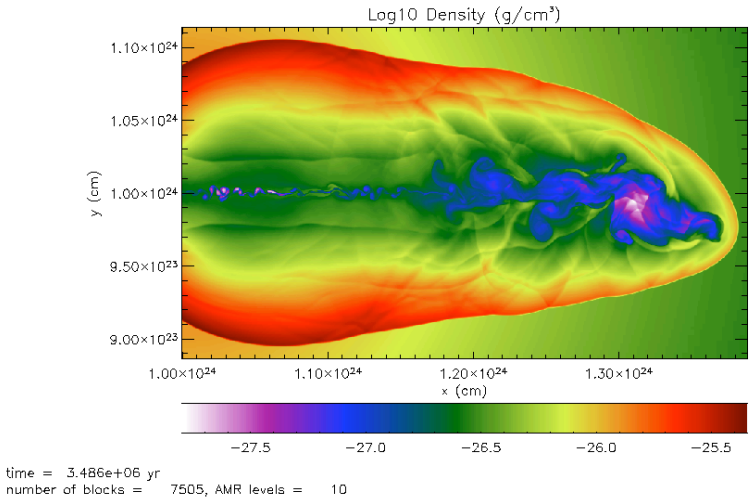

Figure 1: Morphology of a very fast jet propagating through the intracluster medium, shortly after being terminated.

if necessary.

In this set of simulations, only a small part of the problem described in the introduction was studied. The main intention was to study the effect of different jet powers on the structures formed by the interaction between the jet with the ambient gas. To simplify matters the jet power was not directly linked to the radiative losses and the jet was activated at pre-defined periodic intervals. This was partly because it is still unclear how to properly relate the jet power to the inflow rate of material, and partly because a periodic injection of identical quantities of energy allows a better analysis of the morpholgy of the jets than highly variable energy injection.

The simulations were run on IRIDIS 2, one of the University of Southampton's Beowulf clusters. IRIDIS 2 is one of the largest computational facilities in the country and currently consists of more than 800 processors, of which roughly 600 are 2.2 GHz AMD Opterons and 200 are 1.8GHz Intel Xeons. Jobs were typically set to run for a couple of days on 30, or so, processors.

Results

The simulated jets are lower density, than their surroundings, by about a factor of 100-1000, but are assumed to be in pressure equilibrium. This is because the jets would, if over-pressured compared to their surroundings quickly find an equilibrium with their surroundings. The total jet power is also divided between thermal and kinetic components. With this prescription it is possible to investigate the behaviour of a jet that is described by different ratios of kinetic to thermal power.

The jets excavate a cavity in the ICM which is clearly visible, in agreement with observations. The morphology of these cavities depends upon a multitude of parameters. For example, if the jet is dominated by its kinetic power then the cavity will be elongated along the jet axis. As the relative importance of the thermal component increases, the cavity becomes more spherical. Interestingly, such quasi-spherical cavities are frequently observed in the atmospheres of galaxy clusters. This perhaps hints that the thermal and kinetic components of jet power are roughly in equipartition in real jets. The duration that a jet is active for also affects the morphology of the cavity.

These simulations reveal that the jets which produce cavities that most resemble those observed in real clusters are those which are inflated by relatively slow outflows, where the kinetic and thermal jet components are in equipartition. For example, outflows with velocities of a few $\times 10^8 \mathrm{cm\,s^{-1}}$ readily produce objects that resemble the 'spherical cap' bubble observed in the Perseus cluster. Perhaps this could imply something about the fuelling mechanism, or that the jet velocity is reduced due to the comparatively dense atmospheres which envelope them in galaxy clusters.

The morphology of the structures formed by the jets is also reassuringly similar those seen in laboratory experiments. In such laboratory experiments dye is injected into water and forms vortex sheets. If the numerical resolution of the simulations was sufficient it is likely that vortex sheets would have been visible.

Since these cavities are less dense than their surroundings they rise buoyantly. Under normal circumstances one would expect these cavities to be rapidly shredded by Rayleigh-Taylor and Kelvin-Helmholtz instabilities since their is no surface tension (provided by magnetic fields, or otherwise) in these simulations. This is indeed the case when cavities are placed ad hoc (without being inflated by a jet) into identical surroundings as these. However, something about the inflation process seems to have stabilising on the surface of the cavity. One possibility is that the backflow of material away from the leading surface of the jets,

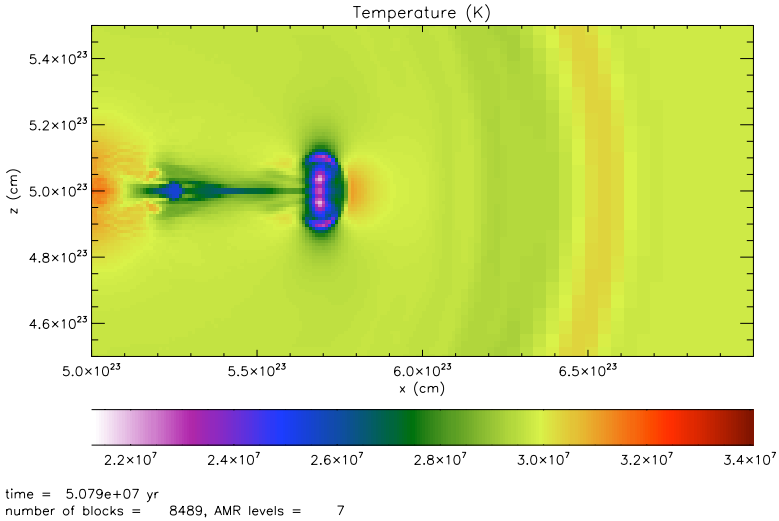

Figure 2: Morphology of a cavity inflated by a relatively slow jet. The cavity ascends at approximately the local buoyant velocity.

after it interacts with the ICM, reduces the relative velocity of the cavity to the ICM thus reducing the rate at which K-H instabilities can grow.

Summary

Galaxy clusters are some of the most impressive structures in the Universe, and are maintained in a quasi-steady state by physical processes which are still relatively poorly understood. This is partly because the very nature of the problem is far beyond our everyday experience. In addition, these objects can only really be studied using detailed numerical models. Only relatively recently has computing power caught up sufficiently with our requirements so that we can make really meaningful numerical studies into these environments. For example, until a few years ago many studies of these objects were performed in only one or two-dimensions.

These objects are also excellent laboratories for investigating our models of how jets from an AGN behave, particularly in the presence of an obstructing medium. As computing power increases we can increase the complexity of the

models to include more complex physics and eventually construct a more complete model of how galaxy clusters are heated.

Dr Edward Pope is currently working in the School of Physics and Astronomy at the University of Leeds and can be contacted by email at `e.c.d.pope@leeds.uk`.

Computational Physics Group News

The Computational Physics Thesis Prize 2006

The Committee of the Institute of Physics Computational Group has endowed an annual thesis prize for the author of the PhD thesis that, in the opinion of the Committee, contributes most strongly to the advancement of Computational Physics. A total prize fund of £1000 will be divided between the prize-winner and the runners up. The number of awards is at the discretion of the Committee.

- The deadline for applications is March 1st, 2007.
- The submission format is a 4 page (A4) abstract together with a citation (max. 500 words) from the PhD supervisor and a confidential report from the external thesis examiner. Further details may be requested from short-listed candidates.
- The submission address is:
  Dr M Probert
  Department of Physics
  University of York
  York, YO10 5DD
  email: mijp1@york.ac.uk
- Please enclose full contact details, including an email address.

Applications are encouraged across the entire spectrum of Computational Physics. The competition is open to all students who have carried out their thesis work at a University in the United Kingdom or the Republic of Ireland, and whose PhD examination has taken place in 2006.

The Computational Physics Thesis Prize 2005

The winners of the 2005 competition were Alex Robinson and Zhongfu Zhou (£500 each).

IoP Computational Physics Group - Student Travel Award

The Computational Physics Group (CPG) of the Institute of Physics (IoP) is pleased to invite requests for partial financial support towards the cost of attending scientific meetings relevant to the Group's scope of activity, as outlined on our web page: http://groups.iop.org/CP/. The aim of the scheme is to help stimulate the career development of young scientists working in computational physics to become future leaders in the field.

To be eligible the applicant should:

- be a full time PhD student;
- provide evidence of acceptance of a presentation (oral or poster) at the meeting in question;
- give an itemised estimate of cost of attendance;
- provide a letter of support from their project supervisor which:
  - ▷ confirms the applicant's PhD student status;
  - ▷ explains the relevance of the meeting;
  - ▷ details the source of the additional funds necessary to attend the meeting.

Applications are invited at any stage in a given year, but will be reviewed by the CPG Committee on a quarterly basis (1st March, 1st June, 1st September, 1st December). Successful applicants will be notified as soon as possible thereafter. Candidates are advised to make their submissions well in advance of the meeting they wish to attend. The maximum support available to any applicant will be £200. The CPG's decision regarding financial support and its level will be final and non-negotiable in all cases.

Successful applicants will be asked to provide a short written report of the meeting suitable for publication in the CPG Newsletter.

For further details, please contact:

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Reports on meetings

Computational Magnetism 2006

13 December 2006, London, UK.

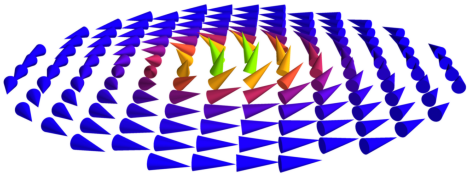
Meeting organised by Hans Fangohr, sponsored by the Computational Physics Group. Co-organised and co-sponsored by Prof Walter Temmerman and the Magnetism Group
A one-day meeting on "Computational Magnetism" ranging from the atomic scale up to length-scales of micrometres was held at the Institute of Physics. The purpose of the meeting was to bring together two communities of computational physicists and engineers in the field: from *ab initio* calculations and from larger length scale approaches such as Heisenberg models and continuum descriptions of magnetism. Interaction and close collaboration between these communities is necessary to move towards multi-scale simulations of magnetic phenomena.

Invited speakers included Dr Robert McMichael from the National Institute for Standards and Technology (NIST) in the US, Dr Uli Nowak (University of York) and Prof Balasz Gyorffy (University of Bristol).

The meeting started after lunch at 13:00 with Prof Gyorffi delivering a talk introducing the *ab initio* methods used in computational magnetism at the shortest length scales. This first session was followed by 4 other talks from Dr Dzidka Szotek (Daresbury, UK), Mr Ian Hughes (Warwick, UK), Prof Ray Bishop (Manchester, UK), and Dr Balazs Ujfalussy (Budapest, Hungary).

Coffee was served during the poster session from 15:00 to 16:00. The second session started with Dr Nowak's talk on Heisenberg models, followed by Dr McMichael's talk on Micromagnetics. Further speakers in this session were Dr Thomas Fischbacher (Southampton, UK), Dr Wyn Williams (Edinburgh, UK) and Prof Thomas Schrefl (Sheffield, UK).

The meeting finished with a Buffet Dinner and Drinks Reception (18:00 - 20:00). A group of approximately 15 participants went to visit a pub before heading home an hour later.



The figure shows the equilibrium magnetisation in a small ferromagnetic Ni-disk with a diametre of 100nm. The long range dipolar interaction aims to avoid surface charges; thus the magnetisation aligns with the boundary of the disk. The exchange interaction favours local parallel alignment of neighbouring atomic moments: for this reason the magnetisation points out of the plane at the centre of the disk (otherwise there would be *anti*parallel alignment at that position.

New Models and Hydrocodes for Shock Wave Processes in Condensed Matter

10 - 14 April 2006, Dijon, France.

Report by Matthew R. Farrow, York University.

The rapid advancement of modern computational power has greatly aided the shock-wave research community. Research in this field is still dominated by experiment, but more and more computer simulations are being performed to aid in the understanding of these energetic and sometimes catastrophic events known as shock-waves. "New Models and Hydrocodes for Shock Wave Processes in Condensed Matter" is one of a small number of conferences aimed at the shock-wave researcher. It is held every two years and attracts researchers with backgrounds in both industry and academia, from many different countries (there were 8 countries represented at this conference). My supervisor and I saw this conference as a great opportunity to gain a lot of insight into the field of shock-wave research, particularly as I am in my first year of a Ph.D, researching shock-waves from a Molecular Dynamics simulations approach. I put together a poster for the conference entitled "Simulating Shock-Waves in Aluminium". This was created from my research into using classical potentials to model the interactions between 108 Aluminium atoms. Classical potentials had to be used in place of *ab-initio* simulations as the computational load for the size of the systems to be used was too great for the current level of computers to handle. An empirically determined classical potential known as the Embedded Atom Method was chosen to model the Aluminium interactions and we where pleased to find that not only was the poster well received, but the model we had chosen (out of a number of

possible models) seemed to be the one most of the researchers recognised as the right one to use.

The format for the conference was five days of talks with four hours of presentations in the morning and four hours of presentations after lunch (with coffee breaks!), for four days (the fifth day afternoon was set aside for travelling from the conference). The afternoon sessions were mainly on Numerical Models and so emphasis on these talks will be given here.

The session; "Mechanisms of Shock Wave Processes at the Micro Level" was also very interesting as there where many useful talks, particularly Brad Holian's Overview talk. In his talk, Dr. Holian covered a wide range of topics in shock-wave research- from empirical potentials used to model atomic interactions to the much larger-scale material break up and scattering. A talk in that session that was also very interesting was by T. C. Germann of Los Alamos National Laboratory, USA, entitled "Molecular Dynamics Simulations of Plasticity and Spallation in Porous Single Crystal Copper" it had movies of his group's computer simulations, performed with 300 billion atoms on 131,072 processors of the IBM BlueGene/L supercomputer at Lawrence Livermore National Laboratory.

This conference allowed the interaction with many of the top names in the field of shock-wave research and although the main emphasis was on experimental research, it still provided valuable insight into the current state of the art on the computer simulation research side of the field. I would like to thank the Computational Physics Group for their support.

APS March Meeting, Baltimore 2006

Report by: Nathan Luke Abraham, University of York

This year's March Meeting was my first international conference and my first oral presentation, "A Real-Space Genetic Algorithm for Crystal Structure Determination". I focused on improvements that can be made to genetic algorithms (GAs) when you are considering systems with periodic boundary conditions. An on-line copy of my talk can be found on my website at `http://www-users.york.ac.uk/~nla101/` and a more detailed description of our method can be found in a recent publication [1]. There were also a number of other talks presented at the meeting on similar applications and implementations of GAs which shows a growing interest in this field.

One of the first talks of the conference was an invited talk by Gus Hart on work which has also been published in Nature Materials [2]. This approach searches for the ground state structure of binary alloys in a GA framework. While the method is quite different from my own, there are a number of features of the method that could be incorporated into mine which could improve convergence times. I also had some useful discussions with Gus Hart and his collaborators which gave me a number of ideas that could be used in my research.

There was also a talk by Colin Glass, a PhD student from ETH Zurich, whose research also involves GAs for crystal structure determination. I had not seen a presentation on their method before, and it was useful to talk with him about the USPEX code that he is working on. His results were impressive [3], although he was quite sketchy on the details of the algorithm itself.

As a CASTEP [4]user I found the talk by Peter Haynes on the linear scaling ONETEP code [5] very interesting, especially in the use of *periodic cardinal sine* or *psinc* functions as a basis set. This allows the method to have the localisation required and avoids problems associated with the use of Gaussian basis sets.

Looking to the future of large-scale computational simulations, Francois Gygi's talk, "Large-Scale First-Principles Molecular Dynamics Simulations on the Blue-Gene/L Computer", described the performance of the Qbox code on up to 65536 processors. His talk also outlined the importance of decomposition schemes in attaining peak performance in large-scale parallel computations. In this case, up to 86 % of parallel efficiency was achieved.

Another interesting talk was by Tadashi Ogitsu: "Boron: do we know the ground state structure?". This talk described a simulated annealing search for the ground state structure of this element, which has a non-integer number of atoms per unit cell (320.1 in the hexagonal unit cell). Boron itself has one of the most complicated crystal structures, which are based around 12-atom icosahedra.

I also found that one of the most interesting talks was one of last, "The scaling laws of human travel - A message from George" by Dirk Brockmann. The data presented here was published in Nature [6] and showed how a new power-law could be derived that described human travel, based on data obtained from the `wheresgeorge.com` website [7].This is a website that was set up to track $1 bills as they travel across America in peoples wallets. This approach takes account of all forms of human travel and not just plane travel as previous studies have done.

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XXV Dynamics Days Europe 2005

25–28 July 2005, Technische Universität Berlin, Germany.

Report by: Nick McCullen (Manchester Centre for Nonlinear Dynamics University of Manchester)

Dynamics Days 2005, listed as a Europhysics Conference by the European Physical Society, was hosted this year by the Technical University of Berlin, and over 350 people attended this annual multidisciplinary gathering.

Nonlinear dynamics has grown over recent decades to take in a wide variety of fields in the physical sciences, including physics, mathematics, computing, chemistry, engineering and biology. This was reflected in the impressive diversity of topics being presented at the meeting. From talks on granular materials to presentations on the role of synchronisation phenomena in epilepsy, there was new insight to be gained by even the most battle-worn professor.

Having said that, it is a shame that many speakers seem to lose sight of what their audience will find interesting and instead concentrate most of their allotted time discussing technical details. Given the 20–30 minute time restriction, they often end up rushing the actual results, which are the most important and interesting part of any work. This led to some talks overrunning, causing disruption to the plans of those wishing to visit a variety of parallel sessions.

Of all the talks, my personal favourite was one on the control of noise induced oscillations by Dr. Natalia Janson. Not only was this related to my own

work, involving systems of nonlinear oscillators, but the talk was very clear and insightful. This left me lamenting the shortage of female speakers at this and other conferences - a symptom of the continuing and regrettable male dominance of physics in general. I have found that, on the whole, the much talked about communication skills of women can produce clearer and more interesting presentations.

However, the main benefit of international conferences is to provide the opportunity for people to meet their peers in the field, and Dynamics Days was no exception. I had the opportunity to chat to a variety of people both formally at the poster sessions and informally at the social events.

There were two poster sessions, each split into two rooms due to the large number of people presenting at this year's meeting. Despite being placed in the less frequented of the two venues, my poster on "Determining the degree of predictability of hyperchaotic systems from time series" received attention from a variety of people, and generated some interesting discussions with people studying related topics. I found the experience to be edifying, especially being questioned on aspects of my work which I had not previously appreciated. I also had the opportunity to discuss with other presenters some applications of nonlinear dynamics to other fields which I found to be fascinating and insightful.

The social programme consisted of an afternoon boat trip around the historic heart of Berlin followed by a barbecue buffet meal in the evening. These proved to be not only very enjoyable and relaxing, but also ideal for discussing a variety of topics in a more informal way with fellow researchers. I was able to compare PhD and conference experiences with other postgraduate students and also indulge in discussions about the wider interests of my research group in Manchester.

All in all I found the conference to be rewarding and interesting, and was pleased to have had the opportunity to attend such a major event in the nonlinear dynamics calendar. I will certainly be looking forward to the next time an event such as this takes place. I am very grateful to the Institute of Physics Computational Physics Division for their generous financial support towards my attending this conference.

NATO-ASI summer school on magnetic Nanostructures and Spintronics

3–14 July 2006, Catona, Italy.

Report by: Giuliano Bordignon (School of Engineering Sciences, University of Southampton

The NATO-ASI school on magnetic Nanostructures for Micro-Electromechanical Systems and Spintronics Applications was held at Regent Hotel in Catona, Italy, from the 2nd to the 16th of July.

Concerning the program of the school, the talks covered a wide range of magnetism-related topics, with the participation of students and lecturers from disciplines such as physics, engineering, chemistry and biology.

The program started with an introduction by Dr. Dominique Givord (Laboratoire Louis Néel) and Dr. Giorgio Bertotti (IEN Galileo Ferraris) to the properties of magnetic materials and the concepts at the base of the magnetisation dynamics in the micromagnetic theory. Although some arguments were well-known by the audience, the analysis of the LLG equation with the spin transfer term arose a rich set of questions and their discussion turned out to be quite contributive to my PhD project, which involves the development of a software package for micromagnetic simulations.

At the end of the first day I was therefore pleased to attend the school, and the following days happened to be as good as that one. In fact we had talks from distinguished lecturers such as Dr. John Slonczewski (IBM Research Division), the father of the theory describing the magnetoresistance and spin transfer torque effects, and Prof. Andrei Slavin (Oakland University, Michigan), who showed how a spin-polarized current in magnetic multilayers can generate standing waves at microwave frequency.

The theoretical sessions of the school were combined with more experimental and industrial-oriented lectures, where fabrication processes and applications of magnetic devices were analysed from different points of view. Among the others, I particularly enjoyed the lectures of Prof. Leon Abelmann (Twente University) and Dr. Thomas Thomson (Hitachi Research Center), whose talks were focused on magnetic recording media. They showed how hard disks manufacturers see the Moore's law for storage, which states the doubling of data density on a recording media every 18 months, as an increasing challenging benchmark and pointed out possible ways to face it in the near and far future. So, beside the use of patterned media coupled to thermally assisted recording, the most likely

in the near future, they reported approaches such as the use of cantilever arrays for thermomechanical recording on harmonica drives and the fascinating idea of a cluster of wireless actuators walking on the media surface to read and write data.

This last idea was somehow supported by the lectures of Prof. Orphee Cugat (LEG/CNRS) and Dr. Martin Gijs (LNS/EPFL), who presented a survey of actuators, generators and sensors at micrometre scale and showed how the scaling of these devices in the last few years permitted to design remarkable tools for applications in micromechanics, biology, telecommunications and lab instrumentation.

For whom (like me) not very familiar with magnetic imaging techniques, the first talk of Dr. Mathias Kläui (University of Konstanz) on the various apparata used for experimental measures was very instructive, but the most interesting lecture happened to be his second talk, where he described the interaction between spin polarised currents and domain walls. The systems I investigate in my PhD project are in fact related to what he has shown, and the way he combined the results from experimental measures and numerical simulations was a stimulating example for my work.

Concerning the place where the school was held, it was simply outstanding, with the view of Sicily's strait in front of the hotel and the lights of Reggio's promenade at night. Beside that, the organizing committee was superb over all the period of the school, and I am very grateful to the Computational Physics Group of the IoP for the travel bursary I needed to attend to the school.

International School on the Fundamentals of Nanoelectronics, Keszthely, Hungary

27 August – 1 September 2006, Keszthely, Hungary
Report by Lianheng Tong, University College London

The School

The International School on the Fundamentals of Nanoelectroincs took place between 27th August and 1st September 2006. There were total 81 participants, from 33 institutions of various European countries. Most of the people there were part of a large collaboration for researches in nanoelectronics.

The school was used as an annual meeting for the collaboration to present their current results and ideas in fields such as electron and spin transport, ab initio electronic structures simulations, quantum information and the making of nano-devices. All of the presentations were very interesting, and the most relevant to my current project were that of the works based on the ab initio electronic structure simulation codes SIESTA and SMEAGOL, done by the group from Lancaster University.

The school had been a very fruitful experience for me. The atmosphere in the school was very friendly. I met many people working in nano-science, and exchanged many ideas in particular on methods related to ab initio simulations. As a result, I returned to London with ideas of a new and more efficient electron wave-function propagator for the Ehrenfest dynamics. The new propagator is now applied to the PLATO code I am working on (see next section).

The Poster

During the meeting, I presented a poster on my work on the development of a Time Dependent Density Functional Theory code which models excitations in conjugated polymers. Here is a summary of the presented material:

Tight binding Ehrenfest studies on Polyacetylene

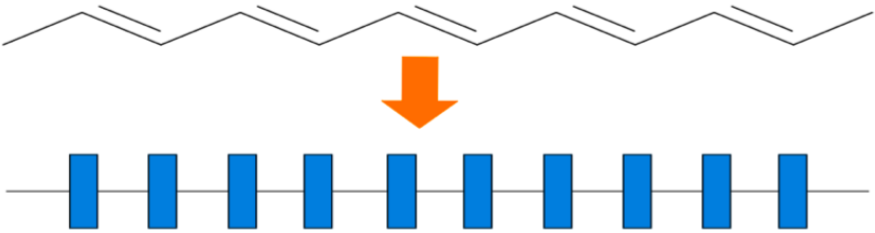
Introduction Conjugated polymers are proposed as potential conducting wires in nanoscale devices. Theoretical studies of the mechanisms underlining these conduction and optical properties of the nano-wires can provide us useful information hard to obtain directly from the experiments. Ehrenfest approximation is a popular method to study the time evolution of complex quantum systems. The main aim of this project is to implement Ehrenfest approximation in a pre-existing tight binding code PLATO.

Polyacetylene has been studied extensively in previous works and it is also the simplest conjugated polymer one can find. Therefore it is an ideal candidate for testing the new implementation.

Ehrenfest Approximation Electrons are assumed to move according to the time dependent Schödinger equation, while ions move according to the Newtonian dynamics:

$$M_i \frac{\mathrm{d}\mathbf{R}_i(t)}{\mathrm{d}t} = -\nabla_i \mathrm{Tr}\left\{r\hat{ho}\hat{H}\right\} - \nabla_i E_{II} \tag{1}$$

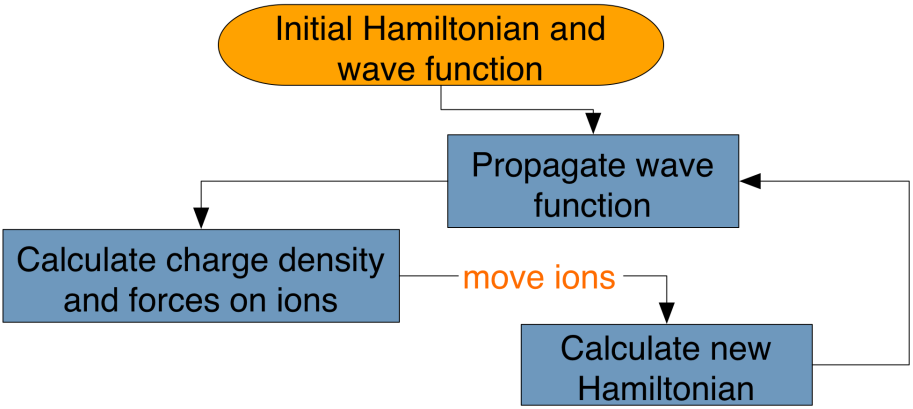
The SSH Model A popular approximation to the structure of polyacetylene is first introduced by Su, Schrieffer and Heeger (SSH) [1]. The polyacetylene chain is simplified by regarding each CH group as one fictitious atom and hence reduces the polymer into an 1-D chain.



The σ bonds are treated as classical springs whiles the π bonds are approximated using first order expansion of the hopping integrals.

Computer Simulation A polyacetylene chain is first relaxed using orthogonal tight binding. Then an electron is excited from the top valence level up to the lowest conduction level. Ehrenfest simulation is then carried out.

The Ehrenfest approximation is implemented in PLATO as shown in the diagram:



The electron propagator is approximated using the Split Operator method:

$$\exp\left(\frac{i}{\hbar}\hat{H}\Delta t\right) \approx \frac{1-\frac{i}{2\hbar}\hat{H}\Delta t}{1+\frac{i}{2\hbar}\hat{H}\Delta t} \tag{2}$$

$$\approx 1-\frac{i}{\hbar}\hat{H}\Delta t+\frac{1}{2}\left(\frac{i}{\hbar}\hat{H}\Delta t\right)^2-\left(\frac{i}{\hbar}\hat{H}\Delta t\right)^3 \tag{3}$$

This approximation is $\mathcal{O}(\Delta t^2)$ accurate, and it is unitary up to $\mathcal{O}(\Delta t^6)$.

Results

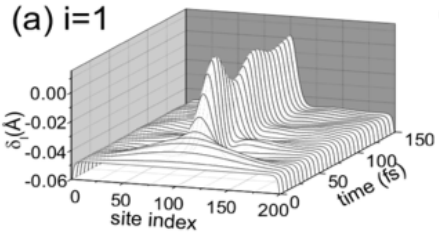


Figure 1. Photo excitation results from An et. al. [2]. It is a plot of the dimerisation (z-axis) against atomic sites and time, calculated using the SSH model.

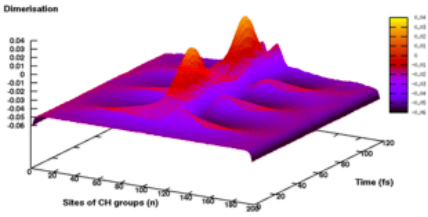


Figure 2. Dimerisation against atomic sites and time calculated from PLATO for photo excitation on a 200 CH groups chain using the SSH model. The time step is 0.001fs.

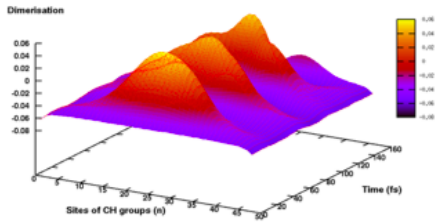


Figure 3. Dimerisation plot calculated from PLATO for photo excitation on a 50 CH groups chain using SSH model. The end groups were pinned and the chain was then relaxed before the photo excitation. The time step is 0.001fs.

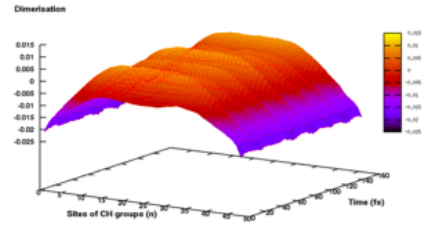


Figure 4. Dimerisation plot calculated from PLATO for photoexcitation on a 50 CH groups chain using the full atomic structure. The structure was first relaxed and then the two end carbons were fixed in position before the photo excitation. The time step is 0.001fs.

Conclusion and future work PLATO reproduced key features from the results of [2], such as the width of the distortion and the time of the first peaks i

dimerisation. There are also clear differences, which still needs to be understood. For shorter chains, the influences from the end boundaries increase. Comparing with the SSH model, the full structures produced more detailed dimerisation structures between the main (SSH) peaks. The apparently flat dimerisation peaks in the full structure result was caused by the fact that the structure was relaxed before the end carbon atoms were pinned. This had to be done to avoid bending effects. A linear scaling DFT code CONQUEST will be available late this year, this will allow the study of longer chains. Possible implementations of a non-adiabatic improvement on Ehrenfest: Correlated Electron Ion Dynamics (CEID) will also be studied.

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International Union of Pure and Applied Physics: Young Scientist Prize in Computational Physics

General information:

- The Award is called "International Union of Pure and Applied Physics Young Scientist Prize in Computational Physics"
- Frequency: triennially, up to three International Union of Pure and Applied Physics [IUPAP] Young Scientist Prizes in Computational Physics will be awarded.
- They will be announced and presented at the annual Conference on Computational Physics (CCP).
- It is intended that one award be made each year. However, in any given year, the selection committee may, at its discretion, may decide not to make an award. If so, multiple awards may be made in the following year.
- It is proposed that the first award be made at CCP2007 in September 2007, in Brussels.

Criteria for selection:

- The recipients of the awards in a given year should on January 1 of that year have a maximum of 8 years of research experience (excluding career interruptions) following their PhD.
- The recipient should be the principal performer of original work of outstanding scientific quality in Computational Physics.
- A previous recipient will not be eligible for another award.

Nomination procedure:

- The awards will be advertised electronically by the C20 Commission on its web page [see www.iupap.org] and elsewhere.
- The deadline for nominations is 1st March.
- Self-nominations will not be considered.
- Nominations shall be made to the Chairman of the C20 Commission by electronic mail [p.h.borcherds@bham.ac.uk] and should include the following:

- ▷ A letter of not more than 1,000 words evaluating the nominee's achievements and identifying the specific work to be recognised.
- ▷ A Curriculum Vitae including all publications.
- ▷ A brief biographical sketch.

The selection consists of the Members and Associate Members of the C20 Commission The selection committee may consult with appropriate external assessors. Type of Awards:

- The Awards will be US$1000 each, plus a medal and certificate to be provided by IUPAP.
- The award money will normally be given as a contribution towards the expenses for attending the CCP.
- The winner will be invited to present a paper at the CCP.

Upcoming Computational Physics Events

Conference on Computational Physics 2007

The Conference on Computational Physics (CCP) 2007 continues the series of the APS-EPS "Physics Computing". It takes place from September 5 to September 8 2007 in Brussels.

Web page: http://ccp2007.ulb.ac.be/Welcome.html

International Workshop on Monte Carlo Codes and 13th UK Monte Carlo User Group Meeting (MCNEG 2007)

The International Workshop on Monte Carlo Codes and 13th UK Monte Carlo User Group Meeting takes place from 26 to 29 March 2007 at the National Physical Laboratory.

Web page: http://www.npl.co.uk/ionrad/training/montecarlo/