Newsletter

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Glassy Dynamics and the Potential Energy Landscape

Newsletter Contents

Figure on cover:

A 'disconnectivity graph', representing a region of the potential energy landscape. Truncated lines show each individual minimum, and the connections between different lines reveal how minima become grouped together at different energies. To produce this graph for a model glassy system we ran a large number of short trajectories starting from the same minimum (shown in red). A more detailed description can be found in the lead article starting on page 1 in this edition of the newsletter.

This Newsletter . . .

Dear Newsletter Readership,

as usual, this newsletter and older newsletters can be found online at http://www.soton.ac.uk/~fangohr/iop_cpg.html, and most URLs mentioned in the newsletter are hyperlinks: clicking on them should take you to the corresponding webpage.

The *main feature* (page 1) of this newsletter is an invited contribution from Dr de Souza who has won the 2008 PhD thesis prize as annually awarded by the Computational Physics Group.

As always, we value your feedback and contributions (email to Hans Fangohr at `fangohr@soton.ac.uk`).

The Computational Physics Group Committee.

Glassy Dynamics and the Potential Energy Landscape

Vanessa K. de Souza

The connection between the properties of glasses and their potential energy surface was originally highlighted by Goldstein [1], and this viewpoint is now well-established [2, 3, 4]. The potential energy of a system is dependent on the interactions between individual atoms and hence varies with the position of each atom, thus forming a potential energy surface or 'landscape'. On a potential energy surface, a minimum is a point from which any small change in atomic coordinates results in an increase in energy. The minimum with lowest energy is known as the global minimum.

Equilibrium thermodynamic properties depend only on the relative potential energies of the local minima and the volumes of configuration space associated with them. However, a description of dynamical behaviour requires further information. Crucially, we need to know about the connections between different minima, and hence the characterisation of transition states, the highest energy point on the pathway between two minima. In this article, we will describe how dynamical properties can be related to the complicated multi-dimensional structure of the underlying potential energy landscape.

Visualising the Potential Energy Landscape

If we have a system of N atoms, the potential energy is described by a $3N$-dimensional function. The potential energy hyperspace requires the height of the surface as an additional dimension, leading to a $3N+1$ dimensional space. Such a high-dimensional surface is rather hard to visualise, and simplifications such as plotting the energy as a function of one or two coordinates can be misleading. Here, we will describe the landscape using 'disconnectivity graphs' [5], which focus on the local minima and the transition states that connect them, rather than trying to visualise the whole landscape.

To construct a disconnectivity graph, such as those shown in Figure 1, we start with a database of minima and the transition states that connect them. At any given total energy, E, we can group all the minima below this energy into disjoint sets (or superbasins) whose members are mutually accessible at that energy. Two minima in the same set are connected by a pathway, i.e. a series of transition states and minima, where the energy never exceeds E. In contrast, the lowest energy path between minima in different sets contains at least one transition state that lies above the threshold energy. The disconnectivity graph displays the energy of each local minimum and their connections to other local minima via the superbasin structure for a discrete series of total energies.
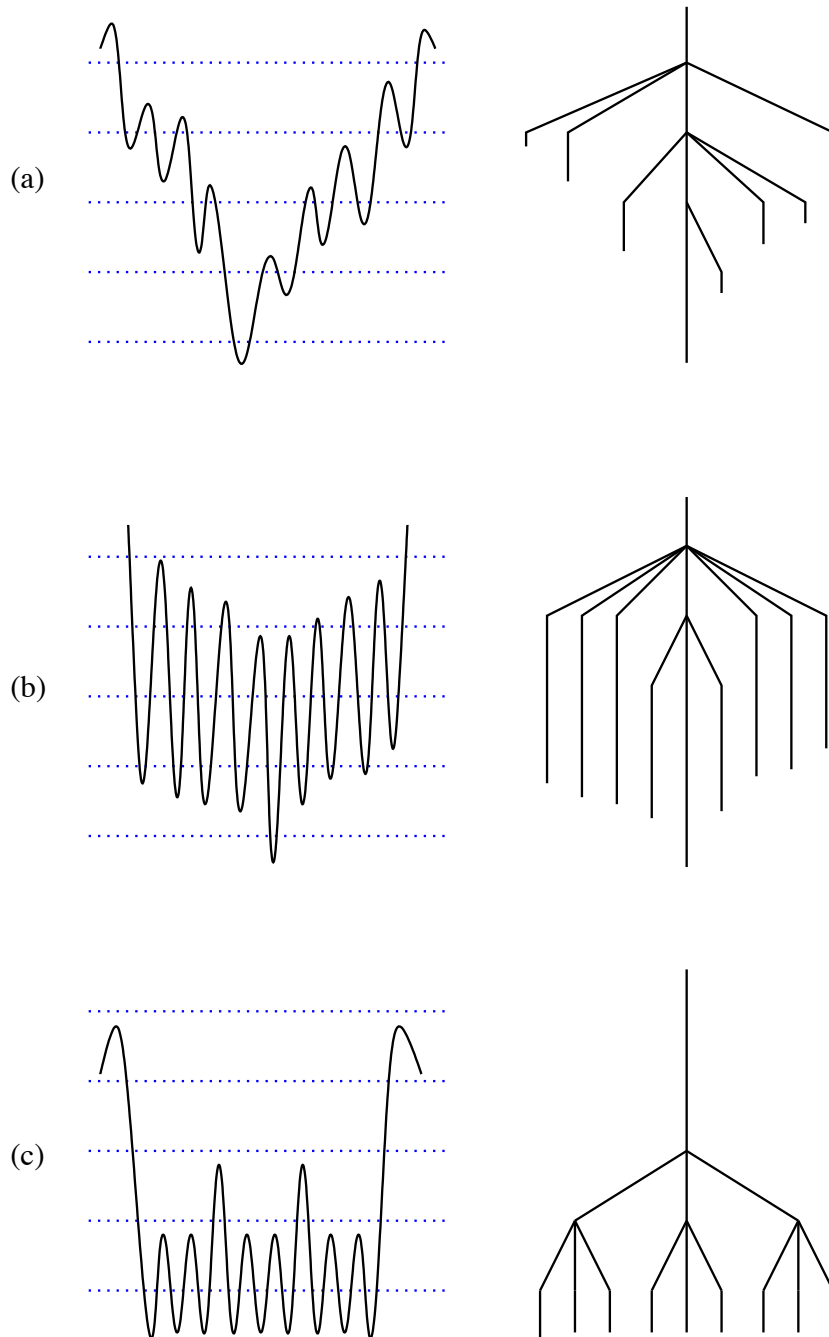
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Figure 1: Each pair of figures shows a one-dimensional potential energy function (left) and the corresponding disconnectivity graph (right). The dotted horizontal lines show the energies at which the superbasin analyses were performed. (a) Palm tree: a well-defined global minimum is reached by traversing low downhill barriers between successive minima where there are relatively large systematic changes in potential energy. (b) Willow tree: the downhill barriers are large in comparison to the energy differences between successive minima. (c) Banyan tree: barrier heights are larger than the typical energy difference between minima and the global minimum is no longer well-defined.

Features of a Disconnectivity Graph

At high energy, there is one superbasin containing all the local minima that can interconvert without restriction (unless the system includes infinite barriers.)

As the total energy is lowered, some transition states can no longer be reached, and the system splits into a number of different superbasins. When displayed on the graph, each superbasin is represented by a point, or node, on the horizontal axis, and the vertical axis corresponds to increasing energy.

Local minima will also become inaccessible, these are shown by truncated lines leading down from the nodes, and eventually, when the energy lies between the values for the two lowest minima, only one superbasin remains, the global minimum.

In a disconnectivity graph, the horizontal axis is usually arbitrary and the order and spacings between nodes can be chosen for clarity. There remains an adjustable parameter in the spacing between the energy levels at which the superbasin analyses are conducted. If the spacing is too large, little topographical information is left, but if it is too small, any coarse-grained structure may be hidden.

Three distinct disconnectivity graphs are shown in Figure 1. Figure 1 shows both the one-dimensional potential energy functions and resulting disconnectivity graphs, formed following superbasin analyses at the energy levels shown by the dotted horizontal lines. Disconnectivity graphs are tree graphs [2, 6], and it is appropriate to describe different shapes by considering the type of tree described by the graph. The 'palm tree' in Fig. 1a corresponds to a function with a well-defined global minimum and relatively small downhill barriers. The 'willow tree', Fig. 1b, has downhill barriers that are larger than the energy difference between minima, but still retains a well-defined global minimum. There is no easily distinguishable global minimum in Fig. 1c, the 'banyan tree', and energy barriers greatly exceed the energy differences between minima.

Landscapes with a palm-tree form correspond to systems that possess an easy-to-locate global minimum and are often good 'structure-seekers' or capable of 'self-assembly'. In contrast, the banyan form is expected to have the slowest relaxation dynamics. The banyan tree has a hierarchical structure, where barriers of different heights separate minima with similar energies. The dynamics of such a system are expected to involve multiple time scales for relaxation, along with power-law decay of correlation functions [7,8]. This structure is typical for glassy systems, and Figure 2 shows an example disconnectivity graph for our model glassy system.

The graph is very complicated, there are no obvious patterns and many levels of hierarchical structure. It is clear that simply elucidating large samples of minima and transition states will not be sufficient to calculate or explain the range of dynamical properties for different glassy systems. It is necessary to simplify the landscape, and
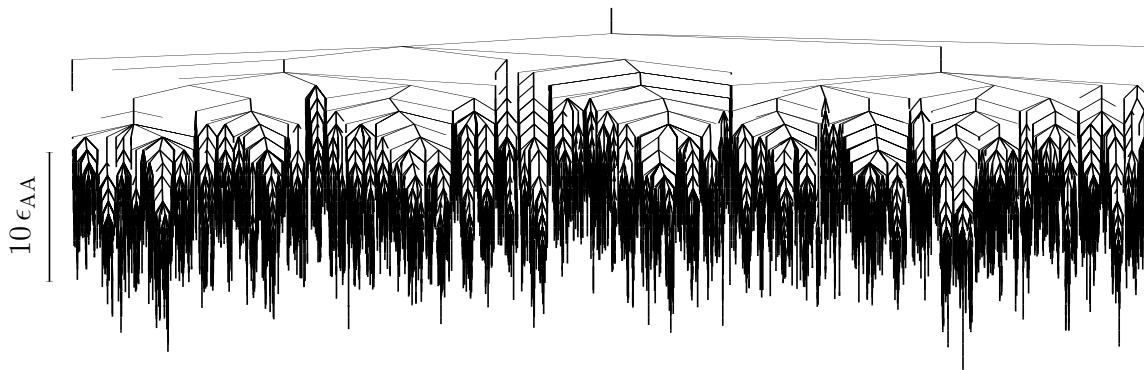
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Figure 2: Disconnectivity graph showing the minima and transition states sampled over a locally ergodic time interval [9] for a 60-atom binary Lennard-Jones mixture. The corresponding stationary point database contains 11474 minima and 13051 transition states. The energy scale bar refers to the total system energy.

focus on the pathways that are pertinent to the system's dynamical properties.
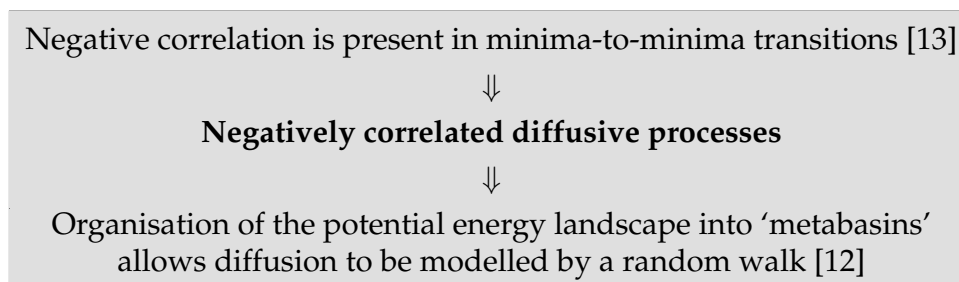
Glassy Landscapes

Studies of glassy systems show that a wide spectrum of potential energy barriers exists [10, 11, 12]. These range from high barriers, corresponding to several pair-well depths, down to processes with very small activation energies. The low barriers reflect the existence of groups of minima between which transitions readily occur. In transitions between these minima, atoms retain their nearest neighbours and the rearrangements are easily reversible with many recrossings occurring in a typical trajectory [13]. These transitions are unlikely to contribute to long-term dynamical properties and because of negative correlation between successive transitions, using information about individual local minima results in an overestimate for the diffusion constant [13].

In an effort to simplify the landscape, the concept of 'metabasins' has been introduced [12, 14]. If all reversals between minima are removed, transitions between 'metabasins' follow an (uncorrelated) random walk and diffusion constants can be calculated. However, this method does not provide an explanation for the values of the diffusion constants. In particular, the diffusion constants for many glasses decrease more quickly with temperature than would be expected for a simple Arrhenius law, super-Arrhenius behaviour [15].

We have found that for temperatures where super-Arrhenius diffusion is evident, it is possible to separate an Arrhenius-like temperature dependence from the true diffusion constant [16, 17]. To obtain the proper value the Arrhenius diffusion can be corrected by including a factor containing the average angle between atomic displacements. On average, displacements were negatively correlated, giving rise to the negative correction factor. A larger negative correlation is evident at lower temperatures

and hence the negative correlation can be directly linked to the increase in effective activation energy, or decreasing diffusion constant at low temperature. We have shown that the negative correlation between displacements is likely to arise from the presence of reversal events, suggesting that we can not simply ignore all such events. Instead, rather than removing all reversals, we wish to remove only those that do not affect long-term diffusion and examine the reversals that might lead to super-Arrhenius behaviour.

The levels of coarse-graining for these different approaches are outlined below:

> Negative correlation is present in minima-to-minima transitions [13]
>
> $\Downarrow$
>
> **Negatively correlated diffusive processes**
>
> $\Downarrow$
>
> Organisation of the potential energy landscape into 'metabasins' allows diffusion to be modelled by a random walk [12]

It has been suggested that the rearrangements in several model glassy systems can be loosely divided into diffusive and nondiffusive processes [11,18]. The nondiffusive (or noncage-breaking) processes occur without changes in nearest-neighbour coordination shells. The diffusive (or cage-breaking) processes involve one or more atoms changing their nearest neighbours; such rearrangements are necessary (but not sufficient) to produce long-term diffusion. If the super-Arrhenius behaviour of long-term diffusion arises due to increased reversals at low temperature, we need to identify these reversals at the level of diffusive (or cage-breaking) moves.

Cage-Breaking

Our first requirement is to identify the fundamental diffusive 'step', to exclude transitions that are not considered pertinent to long-term diffusion, and to demonstrate the validity of these exclusions.

Once an appropriate set of criteria have been defined, cage-breaking transitions can be identified using an analysis of nearest neighbours [19]. An example of a cage-breaking process is shown in Figure 3. A minimum – transition state – minimum sequence is shown, during which the central atom (C), loses 3 nearest neighbours (L) and gains three neighbours (G). We use a binary Lennard-Jones mixture and the two different types of atoms are shown by different colours.

We can show how these cage-breaking and noncage-breaking transitions are manifested within the energy landscape using modified disconnectivity graphs based on Figure 2. The superbasin analysis is performed as usual, but when displaying the
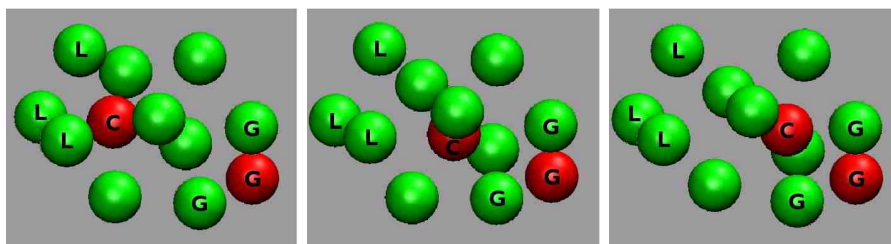
Figure 3: Stationary points on the potential energy surface (minimum – transition state – minimum) for a cage-breaking atom (C) and its nearest neighbours. Three neighbours are lost (L) and three gained (G). The colours (green and red) show the two different types of atoms in the binary mixture.

graph, only connections corresponding to transitions of the chosen type are displayed. This approach causes the graph to be fragmented because some of the transitions required to connect sections of the graph are missing. To highlight this fragmentation, each section is coloured according to its high-energy level limit, following the colour-coding on the left-hand axis, as shown in Figure 4. The colours show the level above which there are no connections to the rest of the graph. Therefore the changes in colour, when traced from the top of the tree downwards with decreasing energy, indicate how the tree becomes separated into different parts when certain rearrangement mechanisms are excluded.

When only the noncage-breaking transitions are included (Figure 4, top panel), the many different coloured sections show that the tree is highly fragmented and, when compared with the original graph in Figure 2, we see that the high-barrier processes are missing. However, for the cage-breaking transitions (Figure 4, bottom panel), the lack of coloured sections shows that the tree is still mostly connected and it also appears to be very similar to the original version. This similarity provides evidence that examining only cage-breaks is sufficient for exploration of the whole landscape and that the exclusion of noncage-breaking transitions from our analysis is valid.

Calculating Diffusion Constants

The second task is to show how long-term diffusion arises from the fundamental diffusive or cage-breaking 'step'.

If diffusion is based on cage-breaking, the only necessary information concerns the atoms undergoing cage-breaks. We can extract the mean-square displacement of a cage-breaking atom and also the rate of cage-breaking events. If we ignore all cage-breaks that are subsequently reversed, this information is sufficient to calculate an accurate diffusion constant. However, it is also possible to include cage-breaks that are subsequently reversed, and to correctly account for their presence using a simple count
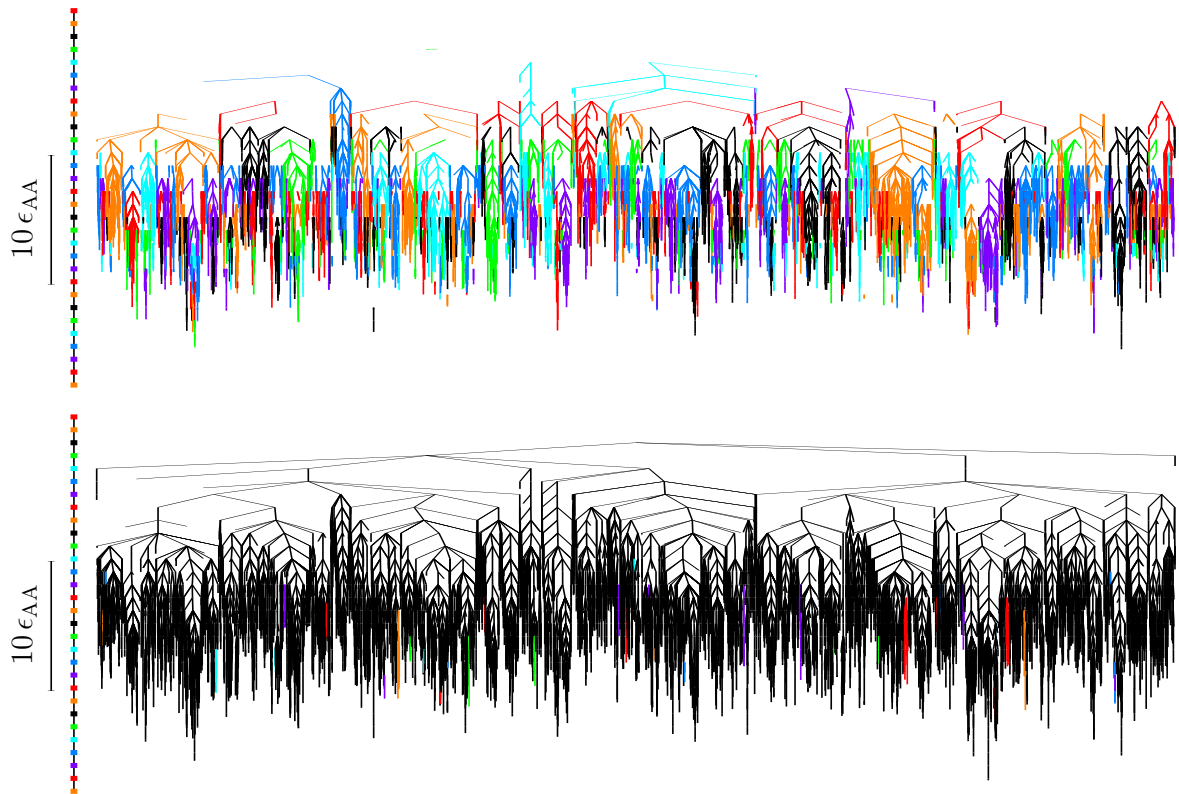
Figure 4: These disconnectivity graphs are an alternative representation of the landscape shown in Figure 2, including only the minima connected by noncage-breaking transitions (top) and only the minima connected by cage-breaking transitions (bottom). The changes in colour show separated branches. The colour of each section corresponds to loss of connection with the rest of the graph at a particular energy level, as shown on the left-hand axis. Following only noncage-breaking transitions does not allow the system to fully explore the landscape, the tree is highly fragmented with many isolated sections. For cage-breaking transitions, the tree is still highly connected and is very similar to the original, including all transition states, in Figure 2.

of reversal sequences which occur in chains of varying length. In this way diffusion is reduced to a correlated random walk of cage-breaking events.

In Figure 5, we show the correction terms (c) required for the calculation of diffusion constants due to reversal chains of different lengths (z), for a range of temperatures. The correction terms oscillate in sign as shown by the solid line for the highest temperature. The number of reversal events increases at low temperature, with lower temperatures shown towards the top of the figure.
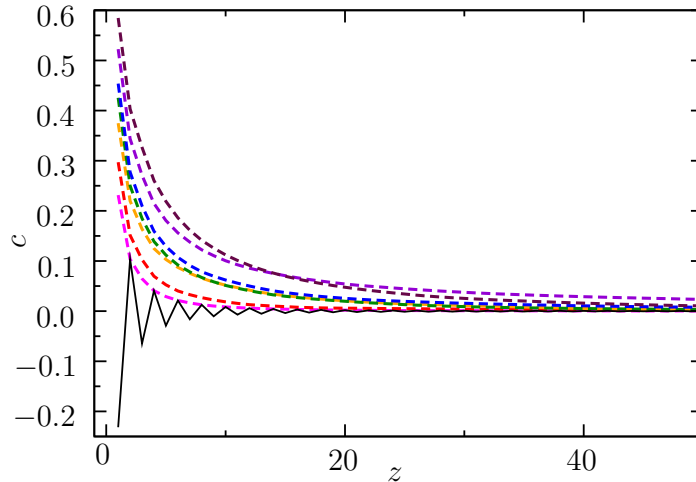
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Figure 5: The number of cage-breaking reversals in chains of varying length, z, is divided by the total number of cage-breaks and shown for a binary Lennard-Jones mixture at a range of different temperatures (dashed lines). The correction terms increase for lower temperatures (towards the top of the figure.) For the highest temperature, the solid black line shows the correction terms with sign included for each value of z. Decay occurs in an exponential manner, as required for long-term diffusive behaviour.

Connectivity

The next task is to determine the cause of the increased cage-break reversals at low temperature, and hence the rapidly decreasing diffusion constants.

One of the strongest candidates for a direct link between the landscape and super-Arrhenius behaviour is a change in connectivity of the potential energy minima. If the number of available escape routes from each minimum decreases at low temperature as expected [20,21], the lack of alternative routes would result in an increased number of reversals and hence cause super-Arrhenius behaviour.

This limited connectivity would not necessarily be visible in a disconnectivity graph representation of the landscape. In the formation of superbasins, the disconnectivity graph shows groups of minima between which the system can move at a given energy. However, there is no information about the time necessary for this interconversion and specifically the number of barriers that would have to be traversed. We can examine connectivity by starting from one particular minimum, assigning velocities at random from a Maxwell-Boltzmann distribution at the correct temperature and running a number of different trajectories.

Figure 6 shows the minima found when 10000 different trajectories are run from the same starting minimum. As we are interested in connectivity in terms of cage-breaking processes, each trajectory stops after the first cage-break of any atom. The starting minimum is labelled in red and noncage-breaking rearrangements are traced

in blue. The two panels show graphs for different temperatures. It is known that at low temperature (right panel), the system explores minima of lower energies [22]. Importantly, following the same number of escape attempts, we also find a considerably reduced number of connections at low temperature. The number of connections also decreases at a higher rate at higher density, tracking the rate of change observed in the diffusion constant. For all temperatures we also find that there are a small number of routes with very high probabilities and these popular routes are found with increasing regularity at low temperature.

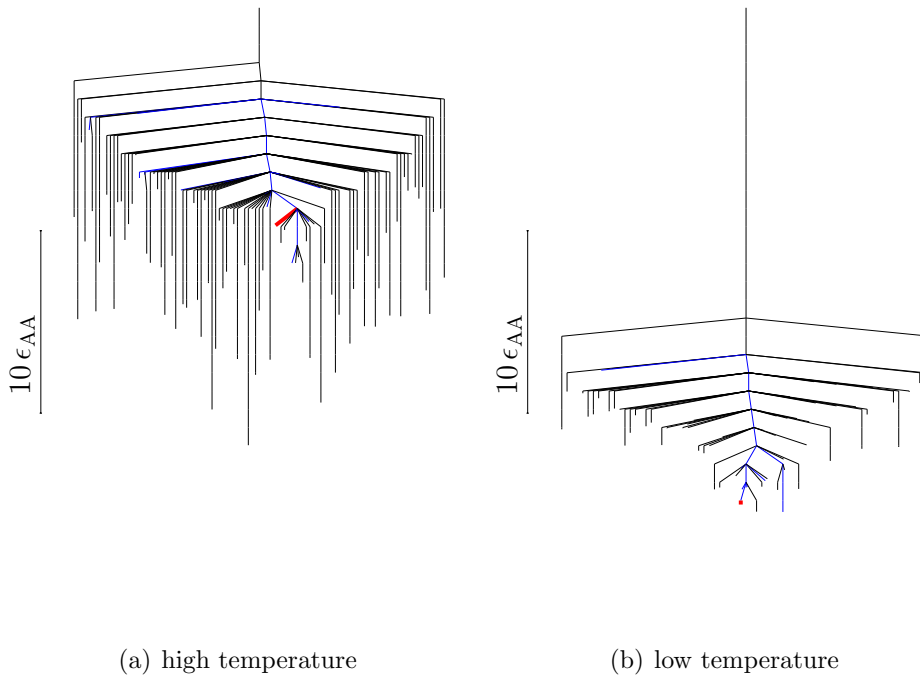(a) high temperature   (b) low temperature

Figure 6: Disconnectivity graphs showing the minima visited in 10000 attempts to escape from a particular starting minimum via a cage-breaking transition. The graphs shown are typical for those found at high temperature (a) and low temperature (b). The starting minimum is labelled in red and noncage-breaking moves are traced in blue.

While these results reflect the expected features of the landscape, there are still unexpected differences in the graph shapes as typified by the examples shown in Figure 6. At low temperature [Figure 6(b)] the graphs could be described as palm trees, and most of the cage-breaking events that allow escape from the starting minimum involve a transition to minima that are higher in energy. Further steps would be required to return to a minimum of equivalent energy to the starting minimum. For high temperatures [Figure 6(a)], the graphs show a willow-tree pattern. Cage-breaking events involve transitions to many different minima at varying energies including many at lower energy than the starting minimum.

Conclusions

Disconnectivity graphs provide a useful tool for visualising multi-dimensional potential energy landscapes. We have presented a direct visualisation of the potential energy landscape for glassy systems, providing a new perspective for a much studied problem, and it is hoped that the viewpoint developed in this work will form a significant contribution to the understanding of diffusion and its connection to the underlying potential energy surface.

The field of glasses and supercooled liquids contains many allusions to the process of cage-breaking. We have provided a clear method for defining such a process (further details can be found in Ref. 19) and demonstrated that an analysis of such processes can be used to study diffusion. Through adapted disconnectivity graphs, we have also shown the significance of such transitions within the potential energy landscape.

A reduction in connectivity between minima at low temperature has been suggested previously [20, 21] as a probable cause for rapidly decreasing diffusion constants. We have demonstrated this effect through direct calculations and also shown that connectivity can be calculated using only small samples of minima, without requiring an ergodic trajectory.

The work described here is a summary of a variety of different ideas developed during my PhD thesis and the descriptions are necessarily terse. Further details can be found in the original articles [19, 23, 16, 17, 24, 9] and I welcome any questions.

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Dr. Vanessa de Souza is the winner of the IoP Computational Physics Group thesis price 2008. Previously at the University of Cambridge, where she completed her PhD under the supervision of Prof. David Wales, she is now working at the University of Sydney, Australia, and can be contacted at vanessa.k.desouza-at-gmail.com.

Computational Physics Group News

Invitation to join

We are always looking for enthusiastic new members to join the Computational Physics Group Committee.

Committee Membership Benefits

> ▷ Meet like-minded colleagues in the field.
> ▷ Arrange (with the help of IoP) meetings of interest to you and others.
> ▷ Help shape IoP policy on Computational Physics.
> ▷ Widen contacts with the Computational Physics Group membership.

Commitments

Meetings are in London, 3 times per year, expenses reimbursed.

Requirements

Member of IoP and Computational Physics Group (which is free to IOP members).

Next steps

Email Geraint Lewis (Geraint.Lewis@velindre-tr.wales.nhs.uk) with an expression of interest.

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

The "International Union of Pure and Applied Physics Young Scientist Prize in Computational Physics" (IUPAP Young Scientist Prize) can be awarded to researchers who have a maximum of 8 years research experience following their PhD.

The annual deadline for applications is 1 March.

See `http://c20.iupap.org/prizes.htm` for details.

The Computational Physics Thesis Prize 2009

The Committee of the Institute of Physics Computational Group offers 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 prize of £250 will be awarded to the winner.

Eligibility and deadline

▷ Applications are encouraged across the entire spectrum of Computational Physics.

▷ The competition is open to all students from a UK institution, whose PhD examination has taken place in 2009.

▷ The submission deadline is June 30th 2010.

Submission format

▷ 4 page (A4) abstract

▷ citation from PhD supervisor (up to 1 A4 page)

▷ confidential report from external thesis examiner (up to 1 A4 page).

Please enclose contact details, including an email address. Further details may be requested from shortlisted candidates.
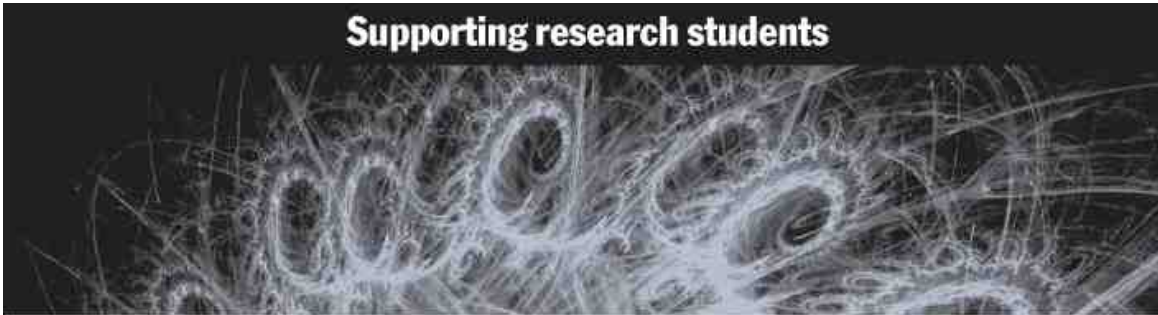
Submission Address

▷ Dr Vera Hazelwood

KTN for Industrial Mathematics

Vera.hazelwood@industrialmaths.net

The Computational Physics Thesis Prize 2008

The Winner of the Computational Physics Thesis Prize 2008 is Dr Vanessa de Souza (previously at the University of Cambridge, now at the University of Sydney, Australia) for her work on Glassy Dynamics and the Potential Energy Landscape, part of which is described in the lead article of this edition (page 1). Congratulations!

IoP Computational Physics Group - Research Student Conference Fund (Travel awards)

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. 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.

Further details can be found at

`http://www.iop.org/activity/grants/Research_Student_Conference_Fund/page_26535.html`

Reports on meetings

British Institute of Radiology Presidents Conference 2009

19 and 20 May 2009, BIR, 36 Portland Place, London, UK

The British Institute of Radiology (BIR) is a multidisciplinary society where those interested in the science and practice of all aspects of radiology (both diagnostic and therapeutic) come together to learn, exchange ideas and to move the subject forward. The BIR Presidents Conference for 2009 was a 2-day meeting focussing on the area of particle radiotherapy, an area which will be of great interest in coming years in the UK.

Radiotherapy delivered with beams of particles such as protons or carbon ions appears to offer considerable advantages over conventional approaches using beams of high energy x-rays. In particular, particle therapy allows treatment with a substantially reduced total or integral dose to the patient, while delivering the same dose to the tumour. This is likely to result in reduced treatment related toxicity, both in the short and long term compared with treatments delivered with x-rays. The reduced long-term toxicity means that proton radiotherapy may become the treatment of choice for a variety of paediatric cancers.

The 2009 conference was the first such collaboration between the BIR and the Institute of Physics, and the meeting was also supported by the Institute of Physics and Engineering in Medicine and STFC The programme was constructed to provide material of interest for the physics research community and the community involved in the clinical practice of radiotherapy, and to stimulate discussion over the 2 days of the meeting. The Support of IoP and IPEM, along with sponsorship from all of the main companies in this field, meant that the very best speakers in the World could be invited. The major sponsor of the meeting (IBA) helped greatly with support for speakers from France who were able to provide important presentations on the approach to particle therapy in their country.

Day one of the meeting focussed on the current and future technologies for particle therapy. All of the main suppliers were represented and the audience heard detailed technical presentations from Siemens, Varian, IBA, Tomotherapy, and Still River Systems. British Research was featured, with presentations from Ken Peach (CONFORM Consortium) and Marco Borghesi (LIBRA consortium). They finished with speakers from France (ARCHADE and ETOILE projects) who explained that in contrast with the UK, it appears that there is little debate in the clinical community on the potential advantages of proton radiotherapy in France, while the role of Carbon ion treatments is considered as an important area of research.

Day two of the meeting addressed some of the future challenges with this new technology, with discussions of radiobiology, imaging and clinical trails. Of particular note was an excellent overview from Michael Goitein, and a summary of the approach being adopted in Heidelburg from Alexandra Jensen. The meeting finished with a round-table discussion of the UK position following a presentation from Dr Adrian Crellin, Chair of the clinical reference panel which coordinates referral of patients for treatment overseas.

The strength of the programme meant that the meeting was very well attended. The BIR lecture theatre was full to capacity (80) for both days.

Stuart Green

Mathematical Aspects of Material Science

23 - 26 May 2010, Philadelphia, Pennsylvania, US

The conference, organised by the Society for Industrial and Applied Mathematics (SIAM), gathered an interdisciplinary group working on the development and application of sound mathematical and computational methods in the scientific study and practical exploitation of materials. Much emphasis was placed on bringing the applied (often industrial) and mathematical community together.

275 international delegates exchanged ideas relating to all application domains of materials modelling. Multi-scale modelling progress and challenges were reported and debated both in the plenary sessions and the parallel symposia. The complete programme is available at http://www.siam.org/meetings/ms10/program.php

Hans Fangohr

Condensed Matter and Materials Physics (CMMP 09)
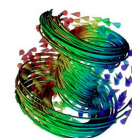
15 - 17 December 2009, Warwick University, UK

Several hundred delegates came together to discuss new ideas about condensed matter physics in the UK and internationally. The CGP co-sponsored two sessions: Nanomagnetism and Computational Electronic Structure and Transport.

The Nanomagnetism session was visited by over 50 people and extra chairs had to be brought in to accommodate them. Jointly chaired by Hans Fangohr and Tiehan Shen from the Computational Physics and Magnetism Group, the first invited speaker was Dr PrivDoz Dieter Suess from Vienna University who explained new concepts for 3d multilayer magnetic recording. The second invited speaker, Prof Quentin Pankhurst from the Royal Institution, demonstrated the state-of-the art use of magnetic nanotechnology in health sciences and therapy. Both speakers have considerable experience in setting up spin-out companies and have shared aspects of this with the audience.

The annual group meeting of the Computational Physics Group took place at the end of the Nanomagnetism session.

The group also sponsored the symposium Computational Electronic Structure and Transport organised by James Annett. Invited speakers at this symposium included Prof. Chris Pickard who gave a lecture outlining exciting new developments in the prediction of crystal structures through random searching.

Delegates of the CMMP2009 in Warwick gather for a coffee break between sessions.

Hans Fangohr

16th UK Monte Carlo User Group Meeting (MCNEG 2010)

12 and 13 April 2010, NPL, Teddington, UK

The 16th UK Monte Carlo User Group Meeting (MCNEG 2010) was held on 12-13 April 2010 at the National Physical Laboratory, Teddington, Middlesex, UK, and organised by Mark Bailey and David Shipley.

The meeting continues a tradition of actually having something of an international flavour, with several of the 40 delegates attending from overseas including the two invited speakers, Katia Parodi (Heidelberg Ion Beam Therapy Centre, Heidelberg, Germany) who gave two talks, Recent and future developments of the FLUKA MC code for ion beam therapy and The role of Monte Carlo at the Heidelberg Ion Beam Therapy Center; and Professor Hooshang Nikjoo (Karolinska Institute, Stockholm, Sweden) who gave a presentation on Radiation track structure, DNA damage, and risk of exposure to ionizing radiations.

Presentations in this meeting were given over four themed sessions, covering Protons and Light Ions; Biological, Protection and Environmental; Radiotherapy and Imaging; and Small Fields and Microdosimetry. It was notable that the FLUKA code was used for several of the presentations and seems to be being used significantly more widely in many applications from radiotherapy to shielding, particle physics to criticality; it has a worldwide community now of over 2000 users. Delegates also had the opportunity to see the new clinical linac facility at NPL as well as some of the primary standards for ionising radiation currently in use. A enjoyable meeting dinner was held at Bar Estilo in Teddington, just a few minutes' walk from NPL, at the end of the first day.

Prizes (kindly provided by the Institute of Physics Computational Physics Group) were offered for the best presentations by students, and we are happy to report that Julien Smeets (ULB, Belgium) won first prize, with his presentation A PHITS-based dose calculation engine to evaluate the effect of inhomogeneities in prostate brachytherapy. Second and third prizes went to Thiansin Liamsuwan (Karolinska Institute, Sweden) and Leena Al-Sulaiti (NPL and the University of Surrey, United Kingdom) respectively.

The organisers are very grateful to the Institute of Physics (Computational Physics Group) and to Elekta plc, who supported the meeting and we hope to have web page available shortly containing all the presentations.

Mark Bailey and David Shipley

Selected Upcoming Computational Physics Events

Fortran in Physics - Its Legacy and its Future?

▷ Monday 7th June 2010 10.00 - 17.00

▷ BCS London Office

▷ http://www.fortran.bcs.org/2010/fortraninphysics.php

▷ Organised by Computational Physics Group (IoP) and BCS - Chartered Institute for IT

The assembled speakers will cover the latest Fortran language standard and demonstrate how the language enables physicists to exploit high-end computing systems to solve today's most challenging problems. Is the future of the Fortran language assured in the physical sciences? Can it survive the rise of alternatives languages and integrated 'mathematical' environments like Matlab and Mathematica? In 2010 the BCS Fortran Specialist Group is celebrating its 40th anniversary.

Attendance is free of charge but please book your place in advance at (http://www.bcs.org/events/registration.

Conference on Computational Physics Trondheim 2010 (CCP 2010)

▷ 23-26 June 2010

▷ Trondheim, Norway

▷ http://www.ccp2010.nohttp://www.ccp2010.no

Condensed Matter and Materials Physics 2010
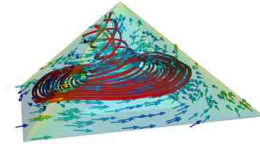
▷ 14 - 16 December 2010, Warwick University

▷ http://www.cmmp.org.uk/

CMMP10, with a wide range of symposia will reflect the breadth of condensed matter and materials physics this series of conferences attracts the highest quality invited and plenary talks, and offers a forum for student presentations. The conference will cover all areas related to condensed matter and materials physics, and their computational modelling.

Conference on Computational Physics Gatlinburg 2011 (CCP 2011)

▷ 16-20 October 2011

▷ Oak Ridge National Laboratory, Tennessee, US

Related Newsletters

The Computational Physics Group works together with other UK and overseas computational physics groupings. We list their newsletter locations here:

▷ Newsletter of the Computational Physics Division of the American Physical Society:

http://www.aps.org/units/dcomp/newsletters/index.cfm

▷ Europhysicsnews newsletter of the European Physical Society (EPS):

http://www.europhysicsnews.org/

▷ Newsletter of the Psi-k (Ψ_k) network:

http://www.psi-k.org/newsletters.shtml.

▷ The bulletin of the Knowledge Transfer Network for Industrial Mathematics, providing information for industrial and academic collaborators on recent results, milestones and opportunities. The full bulletin is available at:

http://www.industrialmath.net/content/news.

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IoP Computational Physics Group links:

▷ Group webpages (http://www.iop.org/activity/groups/subject/comp)

▷ Newsletters (http://www.soton.ac.uk/~fangohr/iop_cpg.html)

Comments about the newsletter, letters and contributions for future editions are welcome and can be sent to Hans Fangohr.