



RESEARCH CONFERENCES

ESF Conference in Partnership with LFUI

Energy Landscapes

16-21 July 2012

Universitätszentrum Obergurgl, Austria

Chair:

David J. Wales, Cambridge University, UK

Co-chairs:

Lapo Casetti, University of Florence, IT

Michael Kastner, University of Stellenbosch, ZA



Conference Highlights

Please provide a brief summary of the conference and its highlights in non-specialist terms (especially for highly technical subjects) for communication and publicity purposes. (ca. 400-500 words)

The 2012 ESF Energy Landscapes Research Conference proved to be a highly successful event in every respect. The conceptual framework of an energy landscape in chemical physics is extremely broad, since it encompasses any system with alternative locally stable states, and the pathways that connect them. Bringing together researchers from very different communities to exchange ideas in apparently disparate fields can be one of the most effective ways of changing the way that fundamental problems are addressed. This Energy Landscapes meeting involved scientists from fields as diverse as atomic and molecular clusters, condensed matter physics including glasses and amorphous materials, physical biology, and fundamental theories of phase transitions and mathematical analysis in terms of the topology of the underlying potential energy surface. In this respect a highlight was certainly the interdisciplinary nature of the interactions, and the way that results in different branches of the subject were able to shed insight into other areas.

One particular highlight for the Chair was the way that different generations of researchers in different fields were able to interact at the Conference. The participation of some key senior figures from different disciplines, along with experimentalists who have inspired some of the cutting edge theoretical research that was presented, was unique in my experience.

Some common themes, which helped to establish connections between different disciplines, included lectures and posters focusing on multi-scale modeling, or coarse-grained representations of complex systems that would be intractable for atomistic simulation. Exploitation of the energy landscape viewpoint as a computational and conceptual framework for understanding and analyzing provided foundations that could be applied in all of the different research fields that were covered. Three principal themes could be identified, name structure prediction, analysis of global thermodynamics, and kinetic descriptions using techniques from rare events theory. Although the systems of interest ranged from models such as spin systems to large biomolecules, including proteins, DNA and RNA, the same issues can be identified in each case. For example, competition between alternative morphologies leads to difficulties in describing the thermodynamic properties, because conventional sampling methods tend to become stuck behind the large barriers that separate competing structures. Interconversion of these competing structures then constitutes a rare event, and prediction of the corresponding time scales is a very active areas of research. Here, most applications have probably been to biomolecules, but the same techniques can be employed throughout atomic and molecular science.

Perhaps one key highlight is the way that new methodology developed for analysis of kinetics and pathways in complex biomolecules is now being applied to study condensed matter. In particular, the complex phenomenology of glassy or amorphous systems clearly requires an understanding of the interplay between processes that occur on very different time and length scales. There were several presentations that demonstrated how new insight has already been gained from such approaches, and the prospects for future research are tremendously promising. The 2012 Energy Landscapes meeting served to catalyse these developments in a extremely helpful way.

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I hereby authorize ESF – and the conference partners to use the information contained in the above section on 'Conference Highlights' in their communication on the scheme.

Scientific Report

Executive Summary

(2 pages max)

The inaugural ESF Energy Landscapes Conference was held in Obergurgl, Austria, from 16th to 21st July 2012. The Chair was Professor David J. Wales (University of Cambridge) with Co-Chairs Professor Michael Kastner (University of Stellenbosch) and Dr Lapo Casetti (University of Florence). There were roughly 80 participants, covering the required age, nationality and gender balances.

Although the ESF contacts for this meeting changed on more than one occasion, the organization was smooth, and feedback between the Chairs and ESF personnel was entirely positive. The choice of venue proved to be very fortuitous, with spectacular scenery complemented by favourable weather, leading to one of the most convivial atmospheres that the organisers have encountered at an international meeting. The travel arrangements for participants to reach this somewhat remote venue were also managed very efficiently by the ESF.

The general impression of the meeting was very favourable, with the mixture of senior key figures and early career researchers in a relaxed environment proving highly productive. The principal objectives of the Conference were to catalyse networking and information exchange between investigators working in very different fields, spanning mathematics, physics, chemistry and biology. The main themes of the meeting were theoretical, but the participation of prominent experimentalists provided important reference points to focus the theory and application of novel methodology.

The energy landscape provides both a conceptual and computational tool for predicting the structure, dynamics and thermodynamics of atomic and molecular systems ranging from nanoscale clusters, through soft and condensed matter, biomolecules such as proteins and nucleic acids, up to much more abstract spin glass models and mathematics of phase transitions based upon fundamental considerations of topology. Theoretical and simulation tools can be developed in a generic way from the underlying potential energy surface, using coarse-grained approaches based upon stationary points. Various other simulation tools can also be applied to any well-behaved potential energy function. Hence new developments of methodology produced in one field can often be applied with only minor modifications to gain new insight into very different areas. The Conference included a number of talks that highlighted such methodological developments, and these have immediately spurred new work within individual groups and in collaborations.

The success of this meeting in bringing together groups working in very different areas suggests a number of opportunities for follow-up activities. These are likely to be organised partly by individual groups beginning new collaborations, but will extend to much more extensive long-term investigations. Smaller workshops that highlight particular opportunities for cross-disciplinary research involving perhaps 20 or 30 participants could be fruitful. The clearest avenues for application of new methods in different fields probably involve the application of novel sampling techniques to condensed matter systems, especially glasses and amorphous materials. Here the opportunity to sample thermodynamic properties in systems with broken ergodicity, and for characterising pathways, mechanisms and kinetic time scales holds the prospect of providing significant new insights. Parallel replica techniques, coupled with analysis of the underlying potential energy surface, and tools from geometry optimisation to locate pathways, will enable rare events methodology to be applied.

One particular highlight of the Conference was provided by the two evening poster sessions, where discussions extended into the late evening, well beyond the timetabled sessions. In fact, similar discussions occurred after dinner on the other days as well. The opportunity to meet participants from different disciplines with common interests, combined with a relaxed atmosphere and inspirational surroundings in the mountains was undoubtedly responsible for this success.

Scientific Content of the Conference

(1 page min.)

- *Summary of the conference sessions focusing on the scientific highlights*
- *Assessment of the results and their potential impact on future research or applications*

The conference sessions were intentionally mixed between all disciplines to highlight the opportunities for transfer of ideas and methodology. Thanks to the support of the ESF it was possible to support a wide range of speakers, from key senior figures to a large number of young untenured researchers at the beginning of their careers.

The meeting began with contributions from two senior figures, namely Peter Wolynes and Austen Angell, who are regarded as pioneers in the fields of free energy landscapes and glasses and amorphous materials. Their talks provided overviews and context for all the related discussions that followed. The next session included presentations on experimental work for DNA, multiscale and coarse-grained modelling, and state of the art results for calorimetric experiments on atomic and molecular clusters. All these themes were reinforced in the next two sessions of the first day, with further talks on biomolecular simulation, and a lecture on liquid crystal-like phases. The latter two sessions also included talks that were focused on methodology for describing global thermodynamic properties, analysing the results of computer simulations, and extracting free energies. Probably the most important result of this first day was the realisation of the cross-disciplinary atmosphere for the Conference, which was one of the most important goals. A poster session followed dinner, and proved to be extremely lively, with exchanges of ideas overheard between scientists from completely different backgrounds.

The second day adopted the same, rather intense, format, starting with presentations on protein folding and novel methodology for characterising pathways between different condensed phases that constitute solid-solid transitions. The condensed matter theme was then elaborated by lectures focusing on crystallisation within the energy landscape perspective, and treatment of non-equilibrium situations. After lunch the topics progressed to spin systems and rare events, with novel methodology described that was inspired by relatively abstract quantum dynamics, but applied to biomolecules. The quantum theme was continued by a presentation on quantum tunnelling, and contrasted nicely with two further contributions on structure prediction. Another lively poster session followed dinner.

The two poster sessions were highlights in themselves. The discussions continued beyond the allotted time in both cases, and simply transferred themselves to the communal areas of the conference venue. These arrangements were clearly a tremendous success, with participants forging new understanding, and in some cases new collaborations, into the late evening.

The third day featured morning sessions and then the afternoon excursion after lunch. The presentations ranged from structure prediction and properties of metal nanoalloy clusters to experimental results for heme-binding proteins. There were also contributions on thermodynamic sampling, supercooled condensed matter, and misfolded proteins associated with neurodegenerative disease. These talks again typified the applicability of energy landscape theory across a tremendously wide range of disciplines, and produced further cross-fertilisation of ideas. Although there was no formal evening session, the after-dinner discussions were just as fruitful and lively as those that followed the two poster sessions.

The final day featured a full programme, culminating in the Reception and Conference Dinner. It was gratifying to note that most people were able to stay for the full programme of the meeting, including the more senior participants, who were a vital source of in-depth knowledge for the early career researchers. The topics covered were again intentionally diverse, and ranged from coarse-grained modelling of DNA, through the mathematics of Riemannian geometry in applications to phase transitions. Several lectures featured discussion of new methodology for sampling complex landscapes, which will be applicable to situations in all of these different areas. The potential impact on future research directions will be very strong for many of the participants. In particular, the use of methodology from different fields, which some workers might have been unaware of, could help to solve outstanding problems. The Conference has certainly had a widespread impact in different areas, as evidenced by a variety of new collaborations that are ongoing.

Forward Look

(1 page min.)

- *Assessment of the results*
- *Contribution to the future direction of the field – identification of issues in the 5-10 years & timeframe*
- *Identification of emerging topics*

The principal objectives of the Conference were certainly achieved. Bringing together groups and individuals from widespread disciplines, where energy landscapes theory is applicable, proved to be very productive. Probably the most important successes were in terms of networking and knowledge transfer between apparently disparate fields of research, spanning mathematics, physics, biology and chemistry. Perhaps the most obvious new opportunities arise from the application of novel methodology developed in one area to problems encountered in a different field. Outstanding examples from the current Conference include structure prediction, global thermodynamic sampling, and kinetic analysis of rare events. Basin-hopping global optimisation was discussed in several talks, and applied to atomic and molecular clusters and biomolecules. In the future, there will be opportunities to use the same approach for soft and condensed matter applications. Similarly, obtaining equilibrium thermodynamic samples for systems with competing morphologies separated by high barriers encounters the “broken ergodicity” problem. This is an issue in glassy and amorphous systems, including spin glasses, and there are clearly opportunities to apply advanced sampling techniques that have been successful for multi-funnel potential energy landscapes in clusters and biomolecules to address such problems. All the novel rare events methods that were described at the Conference are also applicable across disciplines. Sampling glassy systems on appropriate time scales for comparison with experiment is a key issue, and methods based upon coarse-graining of the landscape into stationary points, or minimizing an action principle, are equally applicable to the potentials that arise throughout different fields.

The Conference will make a significant impact on future research directions, in the short, medium and long terms. In the short term, there are straightforward opportunities to exploit techniques developed in one field in different areas. Here the networking and information exchange in the meeting between different groups worked to great effect. Extended discussions after dinner and during and following the poster sessions proved sufficient to cultivate these exchanges. In the medium term, more extensive collaborations will develop from exchange of both established and early career researchers between groups. These collaborations will focus on methodology transfer that requires greater investment of time to adapt computer codes, or refine the relevant theoretical tools. Here, visits of a week or a month to different groups will probably be appropriate, some of which may not require additional funding applications. In the long term, having developed proof of principle, methodology transfer is likely to result in extensive collaborations. This work will be based on a deeper understanding of how fundamental principles are manifested in different fields. In addition, there are likely to be new collaborations between theory and experiment that develop from the mixture of presentations at the Conference. These future directions are potentially just as

valuable as the novel use of new methodology across different fields.

A variety of emerging topics can be identified. Multiscale and coarse-grained modelling of large, complex biomolecules, including mesoscopic systems, is likely to play an increasingly important role. For comparison, much insight has been obtained into colloidal systems using coarse-grained models. The introduction of more versatile and realistic representations of proteins and nucleic acids at a coarse-grained level will facilitate modelling of aggregates such as virus capsids, chaperones, and self-assembled DNA constructs. Other emerging topics include the application of cutting-edge sampling techniques to condensed matter systems, especially glassy and amorphous solids. A detailed understanding of the complex phenomenology of glasses in terms of stationary points of the underlying potential energy surface is under development, and the opportunity to calculate observable properties corresponding to different experimental time scales may resolve a number of outstanding puzzles. Our understanding of how the energy landscapes of spin glass models are organised is also at an early stage. There are numerous possibilities here to develop new insight into these fundamental systems. Another intriguing possibility involves treatment of string theory predictions in terms of energy landscapes.

▪ Is there a need for a foresight-type initiative?

A foresight-type initiative would be very helpful. The most exciting prospects for new research paradigms will surely be obtained by cross-disciplinary activities, which are notoriously difficult to instigate. Funding is required for Conferences and Workshops to build upon the achievements of this inaugural ESF Energy Landscapes meeting, and to foster collaborations. Some of this activity could be relatively straightforward, especially exchange of key researchers and embedding of students in different groups pursuing complementary activities. On longer time scales these initial contacts would lead to much more substantial research projects, which would require funding from the EU or national agencies. The pump-priming of such activities by appropriate initial collaborations is essential. There may be possibilities for funding from Marie Curie Initial Training Networks or Networks of Excellence initiatives, and these should be actively pursued.

Atmosphere and Infrastructure

▪ *The reaction of the participants to the location and the organization, including networking, and any other relevant comments*

The participants were clearly very pleased indeed with the venue and organization. The remote nature of the Conference venue made the whole meeting a great success, and also made ESF transportation arrangements essential. Fortunately this organization and support was of a very high standard, despite a number of changes in the responsible ESF personnel throughout the procedure.

The atmosphere at the meeting was so good that it was constantly remarked upon, including the quality of the food in the restaurant, which was excellent. The only comparable Conferences that I have attended are Telluride workshops and lectures in Les Houches. The treatment of early career researchers was entirely supportive and greatly appreciated, as it has always been at Telluride meetings. The advantage of the ESF Conference was that financial support was available so that more early career researchers could attend. This support made it possible to achieve an age and gender balance that has not been realised at the much smaller Telluride meetings. The opportunity for younger scientists to present their work also distinguished the ESF Conference from Les Houches lecture series.

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None

Date & Author:

18th June 2013 Professor David J. Wales