University of Chicago

Dr. Leonardo E. Silbert
Research Associate

Tel.: +1-773 702 0946
Fax.: +1-773 702 5863
email: lsilbert@uchicago.edu

University of Chicago
James Franck Institute
5640 South Ellis Avenue
Chicago
IL 60637
U.S.A.

Biocomplexity Faculty Search Committee
c/o Prof. Rob de Ruyter
Department of Physics
Swain West 117
727 East Third Street
Indiana University
Bloomington
IN 47405-7105

Dear Sir/Madam

I am applying for a tenure track faculty position recently advertised, to work in areas related to computational modelling of the physical and material properties of complex systems, including biological materials. I am currently a post-doctoral fellow working with Prof. Sidney Nagel, Physics Department, University of Chicago, and jointly with Prof. Andrea Liu, Department of Chemistry and Biochemistry, University of California, Los Angeles.

I enclose a CV that contains my education and research background, a publication list, and contact details of referees willing to support my application. Also enclosed is a research proposal that contains details of proposed projects that I am interested in pursuing upon appointment, and, I feel, would fit well within the structure of the department. The proposal also includes a more detailed summary of my previous research experience. Additionally, I am submitting a teaching proposal that describes my philosophy towards teaching at the undergraduate and graduate level, and outlines of proposed courses I would be willing to develop and teach.

As you will see, my initial education was in theoretical condensed matter physics. However, during the course of my research career I have gained an understanding of problems covering an inter-disciplinary range of research topics ranging from materials science to chemical and mechanical engineering. I have also developed my research in collaboration with colleagues at national laboratories, industrial partnerships, and academic institutions.

I feel that with this wide knowledge base, I can bring a refreshing outlook to contemporary research in your department, not only towards my own projects, but also with the prospect of collaborations within the department, other departments, and outside the university.

Thank you for your time and I look forward to hearing from you soon.

Yours faithfully

Leo Silbert

Research Proposal

Leonardo E. Silbert

Structural and Dynamical Properties of Complex and Biophysical Materials

Systems exhibiting non-equilibrium behaviour and complex, non-linear dynamics are generally known as 'complex' materials. In many cases the standard methods of equilibrium statistical mechanics are not strictly applicable for determining the material properties of such systems. Many everyday examples exist; colloids under flow for applying hand cream, the compaction of granular materials in ceramic component design, and the growth of biological materials during development of the embryo. My education and research in the field of complex fluids have given me an interdisciplinary background that encompasses statistical physics, materials science and engineering, and computer modelling. I intend to apply these approaches to the study of complex and biophysical materials, and investigate the micro-structural and dynamical properties of systems for situations where the competition between interaction length scales and dynamical time scales result in the emergence of interesting phenomena such as self-organization and pattern formation.

Background

My research to date has mainly been concerned with the computational studies of complex systems. I briefly describe these works below.

My PhD project was sponsored by an industrial partner interested in the engineering and characterization of structured materials, during which I regularly visited the research plant to examine product development. To determine how the imposition of flow affects the structure of dense fluids, I undertook a simulation study of concentrated colloidal suspensions to elucidate the micro-structural mechanisms that control their rheology. Experimental techniques for the study of dense colloids are unable to resolve structural features at the particle level in flowing systems. Simulation methods, therefore, offer a way to investigate, at the micro-structural level, why dense suspensions exhibit non-Newtonian rheology and what are the dominating parameters controlling this behaviour. I found that extended force-bearing particle structures - force chains - are a generic feature of concentrated colloids under shear [1]. Identical observations are just now being identified in flows of other types of materials [2]. The competition between flow-induced break-up and the lifetime distribution of force chains controls the rheology, and my results were crucial in formulating a theoretical framework to describe the steady state flow behaviour of dense colloids.

I started my project on granular materials by developing a simulation tool to efficiently study properties of large granular arrays. Flows of granular materials are notoriously difficult to characterize and very much depend on flow geometry and boundary conditions. My work on granular dynamics accurately determined the universal properties of gravity-driven, dense granular flows down a rough, inclined plane [3]. In steady state flow, a balance is achieved between the energy dissipation from particle collisions and the energy input from gravity, leading to a characteristic velocity profile as shown in Fig. 1. Similarly, little is known about the bulk properties of static bead packs due to the difficulties associated with probing the interior of a granular packing. I performed a series of massively parallel computations with up to 128,000 particles to characterize the internal micro-structure of packings and showed how particle friction and inelasticity influence the stress state of the resulting packing [4].

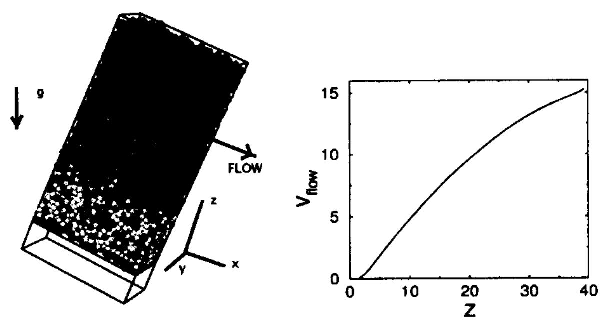

FIG. 1: Left: a computer simulation snapshot of gravity-driven, dense granular flow down an incline tilted 24° with respect to the horizontal. Flow is directed along the x-axis and height is measured along the z-axis. The direction of gravity is given by g. Particles are coloured according to the magnitude of their velocity. Slowest particles (yellow) at the bottom of the pile and faster particles (light blue) at the free top surface. The black particles are the fixed rough base where $z = 0$ and the black frame is the periodic cell. Right: depth-profile of the velocity in the direction of flow.

My present study shows that amorphous systems at zero temperature undergo a transition to 'jamming' that in some features resembles critical phenomena. Comparison of this jamming transition with the liquid-glass transition and the yielding transition in dense fluids indicates there may be some unifying concepts describing their dynamic arrest. I have found that as a disordered system approaches the jamming transition, the number of low-energy modes increases far above what is expected from the classical solid state theory of crystals [5]. The nature of these low-energy modes do not appear to conform to typical phonon behaviour, yet the notion of zone boundaries persists even though the system is disordered. This work is shedding light on the nature of the boson peak and the properties of low-temperature glasses.

Proposed Projects

Introduction

My previous research experience has enabled me to become adept at realizing the interesting physical problems and technological relevance associated with non-equilibrium and complex fluids phenomena. I have developed a suite of computer coding practices and expertise in applying the necessary computational tools, based on sound theoretical reasoning, which form the basis for the research programmes I formulate below. I intend to develop and apply the methods of non-equilibrium statistical mechanics coupled with computer modelling to investigate the micro-structural and dynamical properties of systems where competing length scales and time scales result in the emergence of interesting phenomena such as self-organization and structural evolution.

The research programmes I envisage are concerned with projects dealing with granular materials, biological networks, and modelling techniques to study complex materials. I outline below the main lines of research. Emphasis for a given project will be influenced by the related expertise I find in existing experimental, theoretical, and computational groups, as well as the funding I will seek for these projects.

Phase Behaviour of Granular Materials

Granular materials have often been described as a fourth state of matter because the role of thermodynamic temperature is negligible in comparison with the energy required to displace a single grain, and energy dissipation due to inelastic interactions. Additionally, the phenomenon of size segregation in granular systems do not follow from thermodynamic arguments of phase separation. A collection of granular particles can also exhibit disparate properties simultaneously. For instance, when an avalanche occurs in a sandpile, a thin surface layer of material flows - the 'liquid phase' - yet the bulk remains static - the 'solid phase'. Hence, granular materials are widely recognised as a paradigm for non-equilibrium, dissipative systems [7]. Because of their relative ease of manipulation, studying the dynamics of granular materials can be used as an analogy in describing the properties of dense colloids, foams, super-cooled liquids, and glasses.

With these features in mind, determining the universality of the 'phase behaviour' of granular materials, such as the 'liquid-solid' transition and phase separation, is crucial to formulating and testing a statistical mechanical theory applicable to systems far away from thermodynamic equilibria. Thus the project will involve a simulation study of granular media that are excited, or 'thermalized', driving the system far from equilibrium where the dynamics are inherently non-linear, and examine how varying particle properties such as polydispersity and friction affect the phase boundaries of such systems. Determining the limits of validity of linear response theory would provide insight on how to base the theoretical formulation. This would ultimately lead to possible experimental verification.

Complex Networks and Biological Systems

The nature of force networks in dense colloids and granular materials play an important role in determining the properties of the system. In these cases, the network is locally constrained by the number of contacts between neighbouring particles. An example of a force network for a three dimensional particle configuration is shown in Fig. 2. More recently, networks with different architecture have had an impact in many other fields of science, in particular biophysics, which I intend to explore.

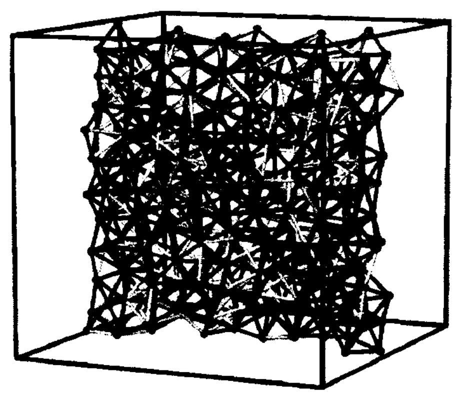

FIG. 2: Force network of a jammed particle system. A slice through the central region of the assembly. Particle centres are shown as small black spheres. Particle-particle contacts are coloured according to the magnitude of the force in the contact with respect to the maximum. In descending order of magnitude: blue, cyan, green, red, and yellow. The black frame denotes the boundaries of the periodic simulation cell. This is similar to recent experimental results for foams [6].

Homogeneous networks, where connections between nodes, or the interactions between particles, are distributed randomly, have been used in a variety of studies from neural network models to gene regulation. However, it has recently become apparent that heterogeneous networks, where nodal connections are power-law distributed - scale-free networks - are ubiquitous throughout nature [8]. It appears that the evolutional advantages of this topology seem to confer to the network functioning.

This research project will investigate the effects that this topology may produce when implemented in models of biological networks. Implementation of a scale-free connection network to a three dimensional physical structure has not been studied, and, as yet, there are no theoretical studies of such systems. By imposing dynamical rules between the connections, it would be possible to study the evolution of physical structures and their connection network, according to the types of rules implemented. Which set of dynamical rules are best suited to describing real systems is still an open question, but can be modelled according to existing or future data of the networks of interest. How the response, inhibition, or enhancement of long-range connections and/or multi-node connections influence regions that are spatially separated is as yet unknown. For example, the network of neural connections are distributed in a scale-free manner within the three dimensional structure of the brain and give rise to collective firing patterns. This project may ultimately lead to a better understanding of problems related to the self-assembly and evolution of biological systems such as the process of morphogenesis.

Modelling of Complex Systems

In general, the properties of complex systems depend greatly on the interactions between the constituent particles. The structural and dynamical response of the system may be greatly affected when one interaction starts to dominate over another. In complex fluids, systems can be classified as either *dry*, as in a granular material like desert sand, or *wet*, like colloidal particles suspended in a solvent, such as blood or paint. Similarly, one can also make the distinction between systems where molecular level interactions are necessary to correctly model physical behaviour and those where such details may be integrated out. Describing the properties of systems lying at the interface of these interacting length scales are particularly difficult to deal with theoretically, but can be studied through computational modelling. The initial core of the project will involve introducing a range of interaction parameters in an effective and efficient manner, and congruent to this would be establishing correct interaction laws for complex particle geometries; dimers, rods, and chains. Current topics of interest are numerous and largely depend on potential collaborations. Some ideas are highlighted below.

In the context of biological materials, the growth and attachment of micro-tubules during the process of cell division have a statistical nature that is just been captured in mathematical models. However, verification of these models is required to understand in better detail the mechanisms that promote or inhibit these processes.

The study of slurries - granular particles suspended in a background fluid - still remains a practical problem from a computational point of view. Correctly implementing granular effects and hydrodynamic interactions in particle modelling techniques has yet to be achieved in an efficient manner. Applications range from the study of geological events like avalanches, mud slides, and erosion, to identifying the mechanisms that lead to material agglomeration and deposition during flow that are relevant to oil exploration and blood flow.

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Teaching Proposal

Leonardo E. Silbert

Introduction

This document provides a summary of my teaching experience and student involvement and presents a philosophy for successful teaching methods, both at the undergraduate and graduate level. I also highlight examples of courses that I am willing to develop and teach.

My education background and research experience have provided me with an interdisciplinary outlook towards topics related, not only to the physics, but also materials science and engineering. This wide knowledge base would allow me to become acquainted with the needs of students with diverse backgrounds from the physical sciences and engineering communities.

Experience

During the course of my research career, I have been involved in various supervisory roles for undergraduate and graduate students as well as high school outreach programmes. I performed as a supervisor in one-on-one tutorial sessions for students taking first and second year undergraduate physics classes in classical dynamics and quantum mechanics lecture courses at Cambridge University. I was a member of a large examples and solutions class session on mathematical methods for theoretical physics students. I also joined a team that introduced research physics to high school students. Recently, I performed as a stand-in lecturer for a first year undergraduate mathematics class at the University of Chicago.

I am also becoming more involved in collaboration and mentoring of PhD students. I have provided theoretical physics advice and computational assistance with a student at UCLA. I am also in continuous discussion with visiting professors and students in experimental physics PhD programmes at the University of Chicago.

Teaching Philosophy and Innovative Methods

Historically, teaching science courses have involved presentation of text book material combined with extensive practice at solving problems. Yet this is not necessarily the most efficient way to project the abstract learning of course material which typically consists of mathematical formulae. It neglects the needs of students to reconcile text book material with real physical problems.

At the undergraduate level, it is essential to present elementary course material in a lucid manner and at a fundamental level for students from a wide background. Motivation for even the most introductory material is necessary to capture the continued interest of students and keep them focused on learning the material. For example, understanding why a particular mathematical formula describes certain physical properties or laws can be achieved by relating course material to everyday experiences. This method of teaching should leave the students with the firm basics of the course material that can be recalled in higher level classes.

For advanced undergraduate and graduate level students, courses can now be presented in a way that begins to challenge the students to think about the problems using the knowledge gained from earlier classes. The teaching method should introduce the language typically used at the research level with an increasing focus on relating content to contemporary research problems. This would bring the students up to a level where they actively participate in research projects.

Below I present some innovative methods to promote student learning inside and outside the classroom.

Student participation and involvement in the classroom develops an open atmosphere where students can feel comfortable asking questions and become accustomed to questioning material they do not understand.

To encourage this approach, the class would be periodically questioned using real-life examples of course material. Grouping students by their seat neighbour, or simply a count of hands to a question would promote this method of teaching. Students would also be encouraged to think about course material outside the classroom and provide feedback for the teacher to explain some problems.

When appropriate, in-class demonstrations with an emphasis on student participation to help explain certain aspects of class material would also be introduced.

With increasing access to the internet, course material and problems solutions would be made available on class web sites.

This provides students with the opportunity to become more familiarized with the use of computers in a scientific and learning context.

Additional material such as more advanced lecture notes, further text book recommendations, and research literature references would be available for the more interested students and particularly for students participating in research projects.

Provided course material is presented in an interesting manner, students will be motivated to solve problems and challenge there own understanding, rather than see them as laborious exercises without meaning. Providing students with problems through in-class examples and homework assignments is valuable in testing the aptitude for students to learn on their own and their ability to continue into research projects.

Course Proposals

Below I provide brief summaries of courses that I would be willing to initiate and develop for teaching.

Scientific Computer Programming

Introductory course in computer programming for scientific purposes at a level that would be accessible to first year undergraduate level of any background and structured to be immediately applicable. Some of the classes would, preferably, be taught in a computer laboratory, or equivalent, for a direct, 'hands-on' approach. Homework assignments would be based on learning by example and some computer laboratory time would be essential.

Computer language teaching of FORTRAN and C would be the basis of the course. Simple computations and data analysis methodology would follow once the basics of the languages have been presented. An introduction to software packages for data plotting would also form part of the course.

Statistical Mechanics and Computer Modelling

Knowledge of statistical mechanics and classical dynamics are a prerequisite to any form of scientific research related to materials. Many classical simulation methods assume a fundamental understanding of these subjects.

An overview of classical dynamics and statistical mechanics in the context of simulation procedures would form the introduction to the course. This would be followed by the core material on classical Molecular Dynamics and Monte Carlo simulation methods. An introduction to parallel computing methods would also be given. The material presented would provide students with the ability to follow current literature and encourage active participation in on-going research projects. This course would be suited to the graduate level and undergraduates with a working knowledge of computer programming.

Complex Fluids

Currently, there is no systematic method for the teaching of complex fluids. However, most modern research in soft condensed matter physics, materials and engineering sciences, and biophysics, involves the study of such systems. Making students aware of the richness of this area of research is the main goal. The prerequisites to the course of thermodynamics, statistical mechanics, and/or some knowledge of the properties materials would suggest that this course be primarily aimed at the advanced undergraduate or graduate level.

An introduction to the physical properties of colloids, polymers, and granular systems in the context of statistical mechanics would form the core material of the course. A basic understanding of the role of interactions, thermodynamic properties, scaling techniques, and rheology would be presented.