Student Conference on Complexity Science

Book of Abstracts
Engineering and Physical Sciences

Brighton 19-22 August 2014

Engineering and Physical Sciences

Wednesday, 20th August 2014

10:00 - 11:00 Simulation Techniques

Simulation techniques: the finite element method

Rebecca Carey, University of Southampton, UK (r.carey@soton.ac.uk)

The Finite Element Method (FEM) is a numerical analysis technique that approximates the solution of boundary value problems (differential equations, which have certain boundary conditions which must be satisfied). It is commonly used in heat transfer and fluid mechanics and it allows for the solution to problems which are too complex for mathematical analysis alone. In this presentation the FEM technique is introduced and explained, with attention paid to problem types that it is well-suited to solving. An example of such a problem is provided to demonstrate the general principles of the technique. Lastly comparisons are made with the finite difference method described earlier in this conference.

Simulation techniques: markov-chain monte carlo methods

Matthew Spraggs, University of Southampton, UK (matthew.spraggs@gmail.com)

I discuss the general principles behind Monte Carlo method as a method for efficiently computing multidimensional integrals, before going on to study Markov chain methods in more detail. I illustrate the generalised form of a Markov chain process, before going on to outline some specific examples in physics, biology and the social sciences.

Simulation techniques: from atoms to planets: "molecular" dynamics as a simulation tool

Chris Cave-Ayland, University of Southampton, UK (C.Cave-Ayland@soton.ac.uk)

Phenomena within complex systems frequently occur not simply in terms of spatial properties but through a temporal dimension e.g. chemical clocks, protein interactions, neuronal signalling. "Molecular" Dynamics provides a robust tool suitable for studying the time evolution of complex systems over a range of length and time scales. This talk will consider what goes into and what can be reasonably expected from a Dynamics simulation, as well as some of the technical considerations.

Thursday, 21th August 2014

9:00 - 10:00 Engineering and the Environment

Stability of power networks under higher penetration of renewable energy sources

Lewis Roberts, University of Bristol, UK (lewis.roberts@bristol.ac.uk)

Increased penetration of renewable energy sources for the generation of electrical power negatively affects the overall stability of the power grid. Using models of synchronisation on the grid we exhaustively study the stability of the smallest non-trivial network, the case of two coupled generators connected to the rest of the grid, under conditions of decreased

inertia. We use a simple coupled oscillator model, the Swing Equation, to study the power grid stability so that we can aggregate generation from similar sources on one node. We develop our stability analysis in the context of Potential Energy Boundary Surfaces and we compare our method to the Critical Clearing Time, a method that is currently used by power engineers. We vary the power output from each machines and the amount of power flowing between the generators in order to investigate conditions for maximising stability.

Exact coherent states in purely elastic parallel shear flows

Toby Searle, University of Edinburgh, UK (T.W.searle@sms.ed.ac.uk)

Parallel shear flows provide a model system for the understanding of the transition to and structure of Newtonian fluid turbulence in incompressible fluids. The turbulent attractor is often thought of as structured by a series of exact solutions to the Navier-Stokes equations. A turbulent flow `pinballs' between these solutions in phase space, spending most of its time very near one or other of these organising structures. So far these structures have been identified in Taylor-Couette, plane shear and pipe flows. One of the first and most important of these exact solutions is the self-sustaining process in plane Couette flow.

Viscoelastic fluid mechanics is complicated by additional nonlinear terms introduced in the constituitive equation for the polymeric fluid stress tensor. As the Reynold's number is reduced and the elasticity of the fluid is increased the nonlinear character of the equations shifts from the Navier-Stokes equation to the constituitive equation. A novel form of turbulence has been discovered in polymeric fluids where the Reynold's number is very low, $Re \leq 1$, and the Weissenberg number (characterising the fluid elasticity) is large.

Using an analogy with the Newtonian self-sustaining process in parallel shear flows, we attempt to construct the purely elastic counterpart for plane Couette flow of polymer solutions. By introducing a forcing term to the coupled Navier-Stokes and Oldroyd-B equations, we observe the formation of purely elastic streaks and consider their linear stability. We find that there exists a previously unrecognised purely elastic analogue of the Kelvin-Helmholtz instability that gives rise to the streamwise waviness of Newtonian coherent structures. I will discuss how this instability might close the cycle and lead to a sustained purely elastic coherent structure.

Optimal strategies for electricity storage

Ellen Webborn, University of Warwick, UK (e.webborn@warwick.ac.uk)

With an increase in the amount of renewable power generation in the UK and a reduction in the proportion of traditional synchronous generators, the task of balancing the electricity grid is becoming increasingly challenging. An energy storage facility could potentially provide multiple types of service to the grid, thus increasing its value beyond what would be possible from price arbitrage alone. In this talk I shall describe my research done in collaboration with National Grid, which models energy storage facilities in order to assess their potential value from price arbitrage, alternatives to infrastructure reinforcement investment, and as providers of grid balancing services.

10:00 - 11:00 Micromagnetics

Micromagnetism and skyrmions: the complex simulation approach

Mark Vousden, University of Southampton, UK (mark.vousden@soton.ac.uk)

This presentation describes the problem that students of micromagnetism face, what a skyrmion is, and how simulations can be used to improve understanding of this complex challenge. The micromagnetics problem is outlined, along with potential applications for its solution. A broken-down description of this problem is provided, showing that the problem can be defined in terms of competing interactions of different types. When these interactions are combined with varying strengths different magnetisation patterns, such as the skyrmion and the helix, are found to emerge. A variety

of simulation approaches to the micromagnetics problem are described, with particular attention to a finite-element method. To conclude the author briefly describes a number of unanswered questions pertaining to the application of this technology, including how the existence of skyrmions depends on the strength of the aforementioned interactions, and the stability of skyrmions in response to perturbation by a magnetic field.

Finite size effects and stability of skyrmionic textures in nanostructures

Marijan Beg, University of Southampton, UK (mb4e10@soton.ac.uk)

Recent research demonstrated that topologically stable skyrmions have the potential to provide new solutions for efficient low power data processing and retrieval. For instance, skyrmions can be as small as a few atoms in diameter, and can be easily manipulated using spin currents five orders of magnitude smaller than those required in conventional magneto-electronics. The geometries of thin film systems in most experimental and theoretical studies are large in comparison to their thickness and close to the limit of thin films that extend to infinity in two dimensions. Of particular importance to the technological application of skyrmionic systems is to understand under what circumstances the skyrmion phase occurs in thin film samples of finite size, which is the main focus of this work. In this work, by using finite element based micromagnetic simulator we show that nanoscale patterned FeGe samples support a new class of incomplete and complete skyrmions without need of external fields or anisotropy (http://arxiv.org/abs/1312.7665). Thin film disk shaped samples with thickness 5 nm were studied for different diameters d and applied external magnetic fields H. We also demonstrate hysteretic behaviour of a single skyrmion in nanostructures, proving that in principle skyrmions in patterned media have unique properties important for data storage and manipulation.

Good vibrations: how to play the magnetic nano-flute

Maximilian Albert, University of Southampton, UK (maximilian.albert@gmail.com)

Magnetic nanostructures are a fascinating example of "real-world" physical systems which exhibit very rich and complex behaviour, due to the interaction of various competing forces at the nano- and micro-level.

One such example is the so-called "spin-torque nano-oscillator" (STNO) which can be thought of as a "magnetic nano-flute". Similar to how a stream of air produces sound waves in a flute when it hits the right resonance, it is possible to excite resonances and standing waves in STNOs by replacing the air with an electric current, creating electromagnetic waves.

In this work we describe the computational aspects of how this property can be used for a novel nano-sensing method where the STNO acts as a kind of "sonar" to detect nearby magnetic nano-particles. By using "functionalised" nano-particles which are coated with antibodies that only attach to a specific substance, this opens up experimental applications for very small, sensitive and versatile detection techniques in "lab-on-a-chip" devices, e.g. to detect tumor markers in a blood sample or environmental polluting agents in water.

11:20 - 12:20 Computational Chemistry

Time correlation function formalism: the case of computational spectroscopy

Valerio Vitale, University of Southampton, UK (vv1c12@soton.ac.uk)

Thanks to the development of new theories and numerical methods, the field of electronic structure theory has undergone a radical change in recent years [1][2]. Contextually, the rapid spread of massively parallel platforms both in the industry and in academia, has precipitated this change. Nowadays, many of the properties of materials can be predicted directly from the fundamental equations of quantum mechanics (QM), or for very large system, a combination of quantum mechanics and classical molecular mechanics QM/MM (for which M. Karplus, M. Levitt, and A. Wershel won the Nobel prize in chemistry in 2013).

This opened the doors to the simulation of a whole range of complex phenomena that were inaccessible before, shedding a new light on critical problems in physics, chemistry, and material sciences, such as superconductivity, drug optimization and biological processes, catalysis etc.

In this work, I will focus on the time correlation function formalism (TCF) applied to ab initio (from first principles) molecular dynamics, which allows to generate accurate and reliable spectra (Infra-red and vibrational) for molecules both in gas and acqueous phase[3][4]. This method naturally takes into account all the anharmonicity arising from a finite temperature, which is not possible with other static methods, providing a better understanding of the structure and conformational transitions that molecules undergo in their native environment. All the calculations have been carried out within the Onetep program, a linear scaling code based on density functional theory. The method has been tested on both small systems in gas phase and very large systems in aqueous phase, such as neutral alanine dipeptide with 500 water molecules, i.e. 1522 atoms, currently the state of art for ab intio molecular dynamics in Onetep. For the latter, about 2000 cores have been used to achieve a trajectory of few picoseconds.

[1] Richard M. Martin. Electronic Structure: Basic theory and Practical methods. Cambridge University Press, 5th edition, 2011. [2] Sidney Redner. Citation statistics from 110 years of physical review. Physics Today, 58(6):49–54, 2005. [3] Mark E. Tuckerman. Statistical Mechanics: Theory and Molecular Simulation. Oxford University Press Inc., 2010. [4] Marie-Pierre Gaigeot. Theoretical spectroscopy of floppy peptides at room temperature. a dftmd perspective: gas and aqueous phase. Phys. Chem. Chem. Phys., 12:3336–3359, 2010.

Lipids - gel to liquid and back again, using meta dynamics to get a leg up in the free energy landscape

Sophia Wheeler, University of Southampton, UK (sophia.wheeler@soton.ac.uk)

Membranes make a cell an autopoetic system. From relatively simple molecules, such as phospholipids, with easily described interactions, membranes self assemble into supra molecular assemblies with rich phase behaviour. Our work focuses on reproducing phase behaviour in silico using a coarse grained forcefield to enable larger systems to be simulated for longer timescales. Phase transitions from "liquid" phases to "gel" type phases have been reproduced for a particular phospholipid. Metadynamics is now being used to drive the simulations over free energy barriers towards "freezing" type events to explore whether such events have not bee seen in previous simulations because the "gel" phase is only meta stable or because the free energy landscape is insufficiently sampled.

Recasting a model atomistic glassformer as an effective system of icosahedra

Rhiannon Pinney, University of Bristol, UK (rp7865@bristol.ac.uk)

The glass transition is one of the greatest open problems in statistical mechanics. One of the mysteries is that at a molecular level, glasses and liquids are seemingly indistinguishable. The exact mechanisms which drive this transition are frequently debated. Sir Charles Frank postulated that five-fold symmetric icosahedra could lead to a change in local structure which might underpin the glass transition. These structures have been shown to play a particularly important role in the glass transition in some binary glass former models. A recently developed topological cluster classification (TCC) algorithm decomposes data into a zoo of clusters – in this case, we seek the icosahedral clusters as described by Frank and ignore all other identified structures for our analysis. By decomposing the full system into an effective system of icosahedra and using techniques from statistical mechanics, we hope to ultimately shed some light on the mysterious nature of the glass transition.