HPC-LEAP Concluding Conference

11-13 July 2018, DAMTP, University of Cambridge

Version of 15:13 on 5 July 2018.

1 Programme

Wednesday 11 July 2018

09:30 – 09:40	N Peake	Welcome
09:40 – 10:10	**C Alexandrou**	**HPC-LEAP**
10:10 – 11:00	**A Kennedy**	**Applying HPC and HPDA Skills to Collaborative Research with Industry**
11:00 –11:30		*Coffee/tea*
11:30 – 12:20	**K Orginos**	**Recent Advances in Understanding the Strong Force**
12:20 – 13:30		*Lunch*
13:30 – 14:20	**C Bekas**	**Cognitive Discovery: How AI Changes the Way We Do Technical R&D**
14:20 – 14:40	E Bennett	Performance optimisation of research codes for the Supercomputing Wales programme: three case studies
14:40 – 15:00	T Nikolov	Asynchronous Linear System Solvers on Supercomputers
15:00 – 15:40		*Coffee/tea*
15:40 – 16:00	G Margazoglou	A Hybrid Monte Carlo algorithm for sampling extreme events in turbulence and stochastic models
16:00 – 16:20	G Tauzin	Study of the Implicit Subgrid scale model within the Entropic Lattice Boltzmann
16:20 – 16:40	J Deasy	Visualisation of Deep Reinforcement Learning in Artificial Intelligence
16:40 – 17:00	J Widdicombe	Numerical General Relativity – Formation of Relativistic Axion Stars
19:00 –		*Conference dinner at Churchill College*

Thursday 12 July 2018

09:30 – 10:20	**P Koumoutsakos**	**Uncertain Predictions and Deep Understanding**
10:20 – 11:10	**S Succi**	**Towards Computational Design of Mesoscale Materials on Exascale Computers**
11:10 – 11:40		*Coffee/tea*
11:40 – 12:00	M Buzzicotti	On the inverse energy transfer in rotating turbulence
12:00 – 12:20	F Milan	Lattice Boltzmann study of droplet dynamics and break-up in generic time-dependent flows
12:20 – 12:40	A Gabbana	Investigating pre-turbulent regimes in graphene samples
12:40 – 13:30		*Lunch*
13:30 – 13:50	X Xue	Effects of thermal fluctuations on a nano-ligament fragmentation
13:50 – 14:10	S Bacchio	Impact of multigrid solvers in lattice QCD simulations
14:10 – 14:30	A Scapellato	Parton distribution functions from Lattice QCD
14:30 – 14:50	S Paul	πN P-wave resonant scattering from lattice QCD
14:50 – 15:20		*Coffee/tea*
15:20 – 15:40	S Cali	Estimate of charm sea effects in QCD
15:40 – 16:00	V Koch	String breaking from Lattice QCD
16:00 – 16:20	A Rubeo	Cutoff effects in gradient flow observables
16:20 – [18:30]		time off for sightseeing [outreach prep.]
18:30 – 19:00	fellows	Outreach event: doors open
19:00 – 19:45	M Wingate	Experiments in Cyberspace
19:45 – 20:30	fellows	Outreach posters & drinks reception

Friday 13 July 2018

09:30 – 09:50	W Lyu	HPC-based molecular simulation investigation on the Protein-DNA recognitions Äìthe effects from post-translational modifications
09:50 – 10:10	T Tarenzi	Open Boundary Simulations of Neuronal G Protein-Coupled Receptors: Towards Drug-Affinity Predictions
10:10 – 10:30	V Bolnykh	Massively Parallel QM/MM Interface
10:30 – 11:00		*Coffee/tea*
11:00 – 11:50	**D Sijacki**	**Cosmological Simulations of our Universe**
11:50 – 12:40	**M Ashdown**	**The Computational Challenge of the Square Kilometre Array**
12:40 – 13:00	M Wingate	Closing remarks
13:00 –		*Lunch & departure*

2 Contributed talks

Abstracts for contributed talks are given below, alphabetically by speaker's surname.

Speaker: Simone Bacchio (University of Cyprus & University of Wuppertal)
Title: Impact of multigrid solvers in lattice QCD simulations
Abstract: We review some results obtained by the application of multigrid methods in lattice QCD simulations. We focus on calculations involving twisted mass fermions and show results for large scale simulations. Namely, we discuss the production of state-the-art ensembles at physical pion masses and how they can be used for obtaining a quantitative description on hadron structure. We will show how the obtained results can probe new physics beyond the standard model.

Speaker: Ed Bennett (Swansea Academy of Advanced Computing, Swansea University)
Title: Performance optimisation of research codes for the Supercomputing Wales programme: three case studies
Abstract: The Supercomputing Wales programme is a strategic investment of £15m by the EU, Welsh Government, and Welsh universities. In addition to procuring new HPC hardware in Cardiff and Swansea, it also provides a pan-Wales team of Research Software Engineers to assist researchers in making optimal use of these machines. In this talk, I will present three case studies of work done by the Swansea University RSE team to assist researchers in getting the most out of HPC. In the first, we took a piece of software for protein folding that spent only 16% of its time doing useful work, and used task bundling to optimise its use of the available processors. In the second, we worked with a piece of in-house Finite Element analysis software, redesigning the parallelisations scheme and bringing it up to near-linear strong scaling. In the third, we have taken a piece of Fortran 77 code for simulating the Thirring model using Domain Wall Fermions and both refactored and parallelised it with MPI, allowing it to tackle significantly larger problems.

Speaker: Viacheslav Bolnykh (RWTH Aachen University & The Cyprus Institute)
Title: Massively Parallel QM/MM Interface
Abstract: Currently, large-scale biologically relevant applications requiring quantum-level description (e.g. simulations of enzymatic reactions or spectral properties) are far too costly. Therefore, the need of a multiscale approach arises. In this framework only a small part which is of particular interest (e.g. the active site) is treated at quantum level (QM part) while the rest of the system is treated by a classical force field (MM part). Using such hybrid QM/MM approach we can drastically decrease the computational effort needed to perform the simulation, keeping the ability to reproduce quantum chemical processes. Unfortunately,

current QM/MM implementations do not scale very well, thus, limiting the accessible simulation timescale. In order to obtain a highly scalable QM/MM code we have decided to use the CPMD code. This is an extremely efficient massively parallel ab initio molecular dynamics software package. It can scale up to few million threads with almost 100% efficiency. Current implementation of the QM/MM method in CPMD has a set of issues, that prevent its usage on large-scale neurobiological applications. First, due to the limited scalability of the MM part the simulation of large systems becomes extremely time-consuming. Then, the choice of a classical force field is limited only to AMBER and GROMOS96 formats. Finally, due to the tight coupling of CPMD routines to the GROMOS96 MM code the user needs to buy a commercial GROMOS96 license in order to be able to run QM/MM simulations.

In this talk we present a new new QM/MM interface using a Multiple-Program Multiple-Data (MPMD) approach with a loose coupling between CPMD and the MM code. Such loose coupling requires the use of an ad hoc communication layer to handle the data transfers between partner codes. Using this strategy we can benefit from the parallelization schemes used both by CPMD and the MM code. Moreover, it also allows us to obtain a flexible and easily extendable framework that can support virtually any kind of forcefield and any MM code. Finally, this strategy circumvents possible licensing issues in case if the MM code is non-free.

Speaker: Michele Buzzicotti (INFN & University of Rome Tor Vergata)
Title: On the inverse energy transfer in rotating turbulence
Abstract: Rapidly rotating turbulent flows are characterised by the emergence of an inverse energy cascade, leading to the formation of large-scales anisotropic vortices. While usually understood as a byproduct of the typical bidimensionalization of rotating flows, the role of the three-dimensional modes is not completely comprehended yet. Indeed, two different mechanisms are known to transfer energy upscale in a turbulent flow. The first is characterised by interactions among triads lying on the two-dimensional manifold, namely on the Fourier plane perpendicular to the rotation axis. The second mechanism is three-dimensional and consists of interactions between triads with the same sign of helicity (homochiral). In order to shed light on this issue, we performed direct numerical simulations of rotating turbulence where the 2D modes are removed from the dynamical evolution. Our results show that while the two-dimensional modes are key to the formation of a stationary inverse cascade, the three-dimensional (homochiral) degrees of freedom play a non-trivial role in bringing energy to the larger scales also.

Speaker: Salvatore Cali (University of Wuppertal & University of Cyprus)
Title: Estimate of charm sea effects in QCD
Abstract: Many simulations of QCD are carried out only with $N_f = 2 + 1$ dynamical light

quarks (up, down, strange). This model has so far provided important results and predictions in Particle Physics and can be considered an excellent approximation of the full theory at energies much below the charm quark mass. However, including a dynamical charm quark in Lattice QCD simulations is important for a better understanding of charm physics and removing the systematic errors which are related to the "quenching" of the charm quark in $N_f = 2 + 1$ QCD simulations.

In this HPC-LEAP project, we investigate the influence of dynamical charm quarks on several physical observables. For this purpose, instead of working in full QCD we study a simplified setup. We simulate two theories: $N_f = 0$ QCD and QCD with $N_f = 2$ degenerate charm quarks. The absence of light quarks allows us to reach extremely fine lattice spacings (0.02 fm $< a < 0.05$ fm) which are crucial for reliable continuum extrapolations. Our main result is a comparison of various quantities such as the hyperfine splitting and decay constants in the continuum limit with a precision that in some cases exceeds 0.5%.

Speaker: Jacob Deasy (University of Cambridge)
Title: Visualisation of Deep Reinforcement Learning in Artificial Intelligence
Abstract: Project aiming to elucidate some of the action-selection mechanisms learnt by deep reinforcement learning agents, using tools from image classification and neuroscience, with the agents neural network acting as the in silico brain.

Speaker: Alessandro Gabbana (University of Ferrara and Bergische Universität Wuppertal)
Title: Investigating pre-turbulent regimes in graphene samples
Abstract: In this work we present realistic simulations of electrons flow in graphene, aiming to determine a viable experimental setup which could be used to trigger and observe pre-turbulent regimes in a hydrodynamic region as close as possible to those within reach of current experimental conditions. We make use of a kinetic formulation enriched to describe the effects of the external electrostatic drive, and to capture the interactions with phonons and impurities. We present simulations in several geometries which could be used to observe fluctuations in the electrochemical potential.

Speaker: Vanessa Koch
Title: String breaking from Lattice QCD
Abstract: In QCD, the static potential $V(r)$ is defined as the energy of the ground state of the system containing a static quark and a static antiquark separated by a distance r. As a consequence of confinement, the energy between the quark-antiquark pair is contained inside a color flux tube, the so called string. As soon as the energy is high enough, the gluonic string connecting the quarks will break due to creation of a pair of light quarks, which combine into

two static light mesons. This so called string breaking provides an intuitive example of a strong decay. Since it is a low energy phenomenon, it is as such not accessible by perturbative QCD, it can only be examined by non-perturbative methods. We investigate string breaking using Lattice QCD, a well-established nonperturbative approach to solving QCD.

Speaker: Wenping Lyu (RWTH Aachen University & The Cyprus Institute)
Title: HPC-based molecular simulation investigation on the Protein-DNA recognitions, Äìthe effects from post-translational modifications
Abstract: Cisplatin is one of the most widely used anticancer drugs. Its efficiency is unfortunately severely hampered by resistance. The High Mobility Group Box (HMGB) proteins may sensitize tumor cells to cisplatin by specifically binding to platinated DNA (PtDNA) lesions. In vivo, the HMGB/PtDNA binding is regulated by post-translational modifications (PTMs). The impact of PTMs on the stability of the HMGB/PtDNA complex is here investigated by enhanced sampling molecular simulations based on the AMBER ff99SB-ILDN and Parmbsc1 force fields. The PTMs turn out to affect the structure of the complex, the mobility of specific regions (including the platinated site), the nature of the protein/PtDNA non-covalent interactions, and the strength of the solvent-solute interactions. In addition, the binding specificity is found in line with the synchrony of the interactions between PtDNA and the proteins. It may account for the experimentally measured greater specificity for PtDNA of the protein isoforms with certain PTMs patterns.

Speaker: Georgios Margazoglou (University of Rome Tor Vergata & The Cyprus Institute)
Title: A Hybrid Monte Carlo algorithm for sampling extreme events in turbulence and stochastic models
Abstract: Extreme and rare events are a defining feature of turbulence but present a severe challenge to standard computational approaches that struggle to systematically sample these events. Here, we present a Monte Carlo importance sampling method that is capable of selectively exploring those remote areas of phase space associated to extreme and rare events. We propose a novel computational approach, based on the path integral formulation of stochastic dynamics, and employ an accelerated Hybrid Monte Carlo (HMC) algorithm for this purpose. As a proof of concept, we investigate the one-dimensional Burgers' equation subject to random noise that is white-in-time and power-law correlated in Fourier space and benchmark our results with standard CFD methods. Furthermore, we present first examples of constrained sampling around saddle-point instanton field configurations (optimal fluctuations) that describe the tails of the probability distribution functions of velocity differences and gradients.

Speaker: Felix Milan (University of Rome Tor Vergata & Eindhoven University of Technology)
Title: Lattice Boltzmann study of droplet dynamics and break-up in generic time-dependent flows
Abstract: We study the behaviour of droplet break-up in generic time-dependent shear flows via a multicomponent Lattice Boltzmann algorithm. Our work can be seen as an extension to studies on the influence of inertia on droplet break-up, whereas we deal with cases of time-dependent droplet break-up, which arise when the temporal rate of change of the shear intensity is of comparable size to the droplet relaxation time. This work is a follow up study to investigations on stable time-dependent droplet dynamics, which were performed via a multicomponent Lattice Boltzmann scheme and compared with the phenomenological Maffettone-Minale model for droplet deformations. Here the main focus is the study of small droplets in a generic hydrodynamical strain field with an additional external time scale, which may be extended to a more realistic model, enabling the study of dilute droplet suspension dynamics under the influence of turbulent fluctuations via a fully resolved Lattice Boltzmann simulation.

Speaker: Teodor Nikolov (Jülich Supercomputing Center)
Title: Asynchronous Linear System Solvers on Supercomputers
Abstract: In parallel environments, asynchronous solvers sacrifice convergence and generality for scalability, fault and latency tolerance. At current scales these methods are viable as preconditioners. They are especially useful when there is inherent load imbalance as they eliminate pro- cessor idle time. Their intrinsic latency tolerance makes them particularly suited for heterogeneous environments as well as future exascale machines.

In this work we present an open-source hybrid parallel library writ- ten in C++(11/14). The library implements asynchronous variants of Jacobi and Block-Jacobi methods, both as standalone solvers and as preconditioners. A general D-dimensional asynchronous distributed stencil matrix-vector product is implemented in the library allowing to test the solvers on variety of systems. The solvers are executed on a number of supercomputers equipped with cutting-edge hardware at the Juelich Supercomputing Center. Various approaches to implementing asynchronous methods on distributed memory machines will be discussed.

Speaker: Srijit Paul (The Cyprus Institute & Bergische Universität Wuppertal)
Title: πN P-wave resonant scattering from lattice QCD
Abstract: This talk focuses on the study of πN scattering in P-wave and $I = 3/2$ where the Δ resonance resides. We use $N_f = 2 + 1$ flavors of tree-level improved Wilson-clover quarks corresponding to a pion mass of ≈ 250 MeV with lattice sizes 2.8 and 3.7 fm, where the Δ is unstable. A combination of stochastic, forward and sequential propagators has been implemented to construct correlation matrices from qqq and $N\pi$ interpolating fields and the

low-lying energy spectrum is determined using the variational analysis. We will discuss the intricacies of the system studied and present the Δ mass and decay width obtained from the Lüscher analysis.

Speaker: Argia Rubeo
Title: Cutoff effects in gradient flow observables
Abstract: Gradient flow observables (gauge invariant composite operators) are easy to measure on the lattice, with high statistical precision; they also have easy renormalisation properties which allow for many useful applications. On the other hand, they have quite large discretisation effects; this problem can be solved by applying the Symanzik improvement programme. We study how to either remove or minimise $O(a^2)$ effects in the case of pure gauge theory.

Speaker: Aurora Scapellato (University of Cyprus & Bergische Universität Wuppertal)
Title: Parton distribution functions from Lattice QCD
Abstract: A key open question of nuclear and particle physics is how nucleons and other hadrons emerge from the interactions of quarks and gluons, known as partons. Parton distribution functions (PDFs) are essential quantities describing the inner structure of hadrons, by giving the probability density to find a parton carrying a given fraction of the momentum of the parent hadron. Traditionally, PDFs are determined through analysis of inclusive deep inelastic scattering (DIS) experiments and are extracted not without ambiguities. We employ the novel approach of quasi-PDFs, proposed by X. Ji in 2013, and extract from lattice QCD simulations, performed at the physical pion mass, the flavor non-singlet u-d distribution functions within the nucleon, with focus on the unpolarized, helicity and transversity PDFs. Our lattice results reproduce the main features of the experimentally determined quantities, showing even an overlap for a range of Bjorken-x values. This first direct non-perturbative evaluation opens a most promising path to compute PDFs in an ab-initio way on the lattice.

Speaker: Thomas Tarenzi (The Cyprus Institute & RWTH Aachen University)
Title: Open Boundary Simulations of Neuronal G Protein-Coupled Receptors: Towards Drug-Affinity Predictions
Abstract: Multiscale molecular dynamics methods allow the coupling of different resolutions in the descriptions of molecular systems. In particular, the so-called Molecular Mechanics/Coarse-Grained approach [1] (MM/CG) was shown to be an effective alternative to all-atom simulations when the absence of structural experimental data and the low sequence identity with templates limit the reliability of membrane protein models. This is the case of G-protein-coupled receptors (GPCRs), which participate in about the 80% of the signaling processes in

the brain and represent the most important family of targets for pharmaceutical intervention [2]. Structural information is lacking for about the 96% of GPCRs. Within the MM/CG scheme, the implementation of the so-called Hamiltonian Adaptive Resolution Scheme [3] (H-AdResS) for the description of the solvent will lead to the simulation of a grand-canonical ensemble in the atomistic region, allowing the calculation of binding affinities in GPCR/ligand complexes where traditional approaches may fail. Towards this goal, we first applied the H-AdResS scheme to biomolecular systems, namely two atomistic proteins in dual-resolution solvent, proving its ability to reproduce structural and dynamical properties of both the protein and the solvent, as obtained from fully atomistic simulations [4]. This paves the way to the use of open boundary simulations for membrane proteins in order to predict ligand affinities.

[1] M. Leguebe, C. Nguyen, L. Capece, Z. Hoang, A. Giorgetti, and P. Carloni, "Hybrid Molecular Mechanics/Coarse-Grained Simulations for Structural Prediction of G-Protein Coupled Receptor/Ligand Complexes," Plos One, vol. 7, no. 10, Oct 19 2012.
[2] D. Wacker, R. C. Stevens, and B. L. Roth, "How Ligands Illuminate GPCR Molecular Pharmacology," Cell, vol. 170, no. 3, pp. 414-427, Jul 27 2017.
[3] R. Potestio et al., "Hamiltonian Adaptive Resolution Simulation for Molecular Liquids," Physical Review Letters, vol. 110, no. 10, Mar 5 2013.
[4] T. Tarenzi, V. Calandrini, R. Potestio, A. Giorgetti, and P. Carloni, "Open Boundary Simulations of Proteins and Their Hydration Shells by Hamiltonian Adaptive Resolution Scheme," Journal of Chemical Theory and Computation, vol. 13, no. 11, pp. 5647-5657, Nov 2017.

Speaker: Guillaume Tauzin (Bergische Universität Wuppertal & University of Rome Tor Vergata)
Title: Study of the Implicit Subgrid scale model within the Entropic Lattice Boltzmann
Abstract: We study the modelling of turbulence implied by the unconditionally stable Entropic Lattice Boltzmann Method (ELBM). In the case of 3D homogeneous isotropic turbulence, we conduct numerical simulations for a wide range of Reynolds numbers. For these simulations, we analyze exact balance relations for energy and enstrophy derived from averaging over a large number of randomly chosen sub-domains of the computational grid. We aim at understanding the behavior of the implied sub-grid scale model and verify a formulation previously derived by using Chapman-Enskog expansion . Finally, we will discuss the properties of the subgrid-scale formulation. These ELBM benchmark simulations are thus useful to understand the range of validity of ELBM as a turbulence model.

Speaker: James Widdicombe (King's College London)
Title: Numerical General Relativity – Formation of Relativistic Axion Stars
Abstract: GRChombo is a new open-source code for numerical general relativity simulations. It is written entirely in C++14, using hybrid MPI/OpenMP parallelism and vector intrinsics

to achieve good performance on the latest architectures. Furthermore, it makes use of the Chombo library for adaptive mesh refinement to allow automatic increasing and decreasing of the grid resolution in regions of arbitrary shape and topology. In this talk I will talk about GRChombo, as well as my recent research on formation of relativistic axion stars that uses this code

Speaker: Xiao Xue (Eindhoven University of Technology & University of Rome Tor Vergata)
Title: Effects of thermal fluctuations on a nano-ligament fragmentation
Abstract: We study the effects of thermal fluctuations on the break-up of nano-ligaments. Our numerical implementation is based on a fluctuating lattice Boltzmann (LB) model for non-ideal multicomponent fluids, including non-equilibrium stochastic fluxes mimicking the effects of molecular forces at the nanoscales. Due to the Rayleigh-Plateau instability, the liquid ligament breaks up into droplets under the growth of disturbances at the interface. Our results show that thermal fluctuations enhance the poly-dispersity of the droplets. Furthermore, we statistically confirm that the presence of the thermal noise accelerates the fragmentation process. The robustness of the observed findings is also corroborated by quantitative comparisons with predictions of sharp interface hydrodynamics. Beyond the practical importance of our findings for nano-fluidic engineering devices, our study also explores a novel application of LB in the realm of nano-fluidic phenomenas.

Speaker:
Title:
Abstract: