



Dansk Fysisk Selskab

Danmarks landsdækkende forening for fysik

Årsmøde 2021

21. – 22. juni

Brogaarden,

Abelonelundvej 40 Strib,

5500 Middelfart

Kom og hør foredrag fra en række yngre forskere i den danske fysikverden: Fra **superkølede væsker** og katalyse **til kvante-devices**, og om bedre **rekruttering** og **læring i Fysik!**



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BOOK OF ABSTRACTS

Monday

PLENARY: The fundamental building blocks of nature

Author: Astrid Eichhorn

What are the fundamental building blocks of matter? What is the microscopic quantum structure of spacetime?

In this talk, I will review recent progress on a new theoretical paradigm that aims at answering these questions. It provides an understanding of the microscopic quantum structure of spacetime and matter based on a new symmetry principle, namely scale symmetry. I will explain the key ideas at the heart of this theoretical paradigm and then discuss how this new theoretical paradigm can be linked to observations and tested with observational data in elementary particle physics and black holes.

SESSION: X-rays and neutrons

Shear-induced ordering in liquid μ -jets revealed by x-ray cross-correlation analysis

Author: Verena Markmann, *DESY*

Co-authors: Felix Lehmkuehler; Gerhard Gruebel

The delivery of colloidal dispersions by microfluidic jet devices has increased scientific and technological interest in the last decades, especially at Free Electron Laser facilities (FEL) [1]. The applications include supercooled liquid production by evaporative cooling of μm -sized droplets [2] and sample delivery schemes for materials sensitive to radiation damage. Free flowing jets as sample environments have the advantage of self-refreshing samples and no solid boundaries, but the inner walls of the nozzles producing the jets inherently apply shear forces to the system. The shear rates in μm -thin liquid jets are in the regime of $\dot{\gamma} \approx 10^5 \text{s}^{-1}$, which is several orders of magnitude higher than in conventional rheometer geometries. For many liquid jet applications the influence of shear on the studied particles or molecules is typically disregarded. However, high shear forces may lead to the formation of anisotropic structure and therefore need to be taken into consideration for time-dependent studies on complex samples such as biological molecules.

This contribution will introduce time- and space-resolved rheology of colloidal dispersions in liquid jets. Therefore, small angle x-ray scattering (SAXS) techniques were applied to scan across and along a μm -thin liquid jet. We observed shear-induced ordering into co-flowing strings of colloidal silica particles and evaluated the asymmetry of intensity and shape of the diffraction patterns by x-ray cross-correlation analysis (XCCA) [3]. For different nozzle sizes and shapes we determined the cessation behavior of the shear-induced ordering and the dependence on the applied shear rate [4,5].

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Ultrafast structural dynamics of AgPtPOP and TIPtPOP

Author: Philipp Lenzen , *Technical University of Denmark*

While optical laser have been available on sub-picosecond timescales for some time, using them to study molecular structural dynamics requires a model of the coupling between energy levels and structure, which is not a given for every molecule. To circumvent this limitation, x-ray scattering techniques have been proposed to resolve atomic movements.

With the construction and improvement of free electron x-ray lasers in recent decades, x-ray sources with unprecedented brilliance and pulse lengths in the sub 100 femtosecond range have become available and thereby allowing such experiments.

Transition-metal complexes have been objects of interest for some time for their photochemical and photophysical properties, making many compounds interesting for applications in catalysis or solar energy conversion. Following excitation they can undergo structural changes accompanied by changes to the chemical properties, which can be resolved with time resolved x-ray solution scattering (TR-XSS).[1]

As the measurements occur in solution to better reflect real chemical conditions, the on short time delays coherent solute signal will be convoluted with adjustments in the solvation cage, heat

dissipation and laser induced anisotropy. These components have to be identified and characterized, in order to fully understand all occurring processes.[2]

The $[\text{AgPt}_2(\text{H}_2\text{P}_2\text{O}_5)_4]^{3-}$ and $[\text{TIPT}_2(\text{H}_2\text{P}_2\text{O}_5)_4]^{3-}$ complexes investigated in this study is a close relative of the intensively studied Pt_2POP_4 [1-3], and allows for deeper insight into the reaction geometry of the system than previous excited state studies. This talk will give an overview on how with the right data treatment and analysis, previously inaccessible sample properties can be extracted out of the terabytes of data measured at large scale facilities.

Acknowledgments

We thank the Danmarks Frie Forskningsfond (DFF) for funding the project and

DANSCATT for supporting the beamtime efforts.

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LINX – Linking Industry to Neutrons and X-rays

Authors: Erik Brok¹; Lise Arleth¹; Martin Schmiele¹; Gregory Smith¹; Martin Alm²

¹ *Niels Bohr Institute*

² *Biomedics Aps*

Neutron and x-ray techniques have a huge potential for solving technological problems for the benefit of society. However, while advanced scientific techniques are invaluable tools for academic research, they are highly specialized and most companies do not have the expertise to take advantage of the opportunities.

LINX is an industry portal, with the goal of enabling Danish companies to benefit from advanced neutron and X-ray techniques. Experts from universities help industry partners identify problems that can be addressed by neutron and X-ray techniques, perform experiments, analyze data, and understand what the results means for their materials or processes. LINX is not just a hub for

bilateral collaborations but a network with mutual trust and inspiration between companies from completely different industrial sectors.

Here, I will give an introduction to the LINX organization and show how we helped Danish company Biomodics understand the structure of their interpenetrating polymer network material for biomedical devices. It is a journey that started with in-house X-ray and AFM experiments, moved on to neutron scattering facilities in France and Germany, and eventually to the reactor in Delft to be able to properly address the question of how two polymer materials are distributed inside a piece of silicone material that has antimicrobial properties and also a potential for drug-delivery.

Application of in-situ time-resolved GISAXS in studying the Solvo-thermal vapor annealing of a homologous series of ABC miktoarm star terpolymer thin films

Authors: sina ariaee, *INM, RUC*; sergey cherneyy, *DTU healtech*; Kristoffer almdal *DTU kemi*; Bo Jakobsen, *INM, RUC*; Nathan barr, *RUC*; florian jung, *TUM*; christine papdakis, *TUM*; Detlef smilgies, *CHESS, Cornell University*; dorthe posselt, *INM, RUC*

Thin films of ABC miktoarm star terpolymers (ABC stars), where three chemically different polymer blocks are linked at a common core, have potentially a very rich phase diagram with occurrence of different types of complex nanostructures. Solvo-Thermal Vapor Annealing (STVA), i.e. interaction with solvent vapor at somewhat elevated temperature, is a versatile method for healing of structural defects and for controlling and manipulating the thin film nanostructure [1, 2].

In the present study, we follow restructuring processes during STVA of three nominally 100 nm thick ABC star films using in-situ time-resolved Grazing Incidence Small Angle X-ray Scattering (GISAXS) with simultaneous Optical Film Thickness Measurement (OFTM). The three ABC stars are composed of poly(isoprene) (I), poly(styrene) (S) and poly(methyl methacrylate) (M) with equal sized I and S blocks while the M block length is varied systematically: ISM2.2 has an arm length ratio 1:1:2.2; ISM3.7 has arm length ratio 1:1:3.7 and ISM5.4 correspondingly 1:1:5.4. The STVA protocol was using toluene vapor at 50C in a custom-made chamber where slow swelling was followed by fast drying with the aim of preserving any ordered nanostructure formed during swelling. The films were studied during STVA with GISAXS scans every 10s, using a x-ray incoming angular range of 0.08° to 0.16°, i.e. distributed around the dry film critical angle (0.12°) for total external reflection.

OFTM results indicate that the larger the M arm contribution in the film material, the less the accessible maximum swelling ratio of the film using the same swelling protocol, consistent with the glass transition temperature of the M arm without toluene being above 50C. GISAXS maps (Fig.1.a-

d), for instance in the case of ISM2.2, revealed that the alternating lamellar structure (LAM – fig. 1a) formed at initial stages of STVA, and was replaced with hexagonally packed core-shell rod structure (HEX – fig. 1b) during film swelling. The achieved HEX structure, however, could not be fully preserved by fast drying.

SESSION: Nuclear and Particle Physics (NICE I)

The FCCee project

Author: Mogens Dam, *Niels Bohr Institute*

The physics case for electron-positron beams at the Future Circular Collider (FCC-ee) is summarized. The FCC-ee core program involves e^+e^- collisions at $\sqrt{s} = 90, 160, 240,$ and 350 GeV with multi-ab-1 integrated luminosities, yielding about 10^{12} Z bosons, 10^8 W^+W^- pairs, 10^6 Higgs bosons and 10^6 $t\bar{t}$ pairs per year. The huge luminosities combined with 100 keV knowledge of the c.m. energy will allow for Standard Model studies at unrivaled precision. Indirect constraints on new physics can thereby be placed up to scales $\Lambda_{NP} \approx 7$ and 80 TeV for particles coupling respectively to the Higgs and electroweak bosons.

Strangeness production in small systems - from revolution to resolution

Authors: Peter Christiansen, *Lund University*; ALICE Collaboration

ALICE measurements show that strangeness production increases with multiplicity in small systems (pp and p-Pb collisions) at LHC energies. This means that one has to give up the idea that a proton-proton collision can be seen as an incoherent sum of parton-parton collisions; an idea that has been central in most proton-proton generators, for example PYTHIA. To accommodate the ALICE results, models have to introduce significant final state effects and the question is now which ones are correct.

In this talk, I will first cover the general results and give examples of models/mechanisms with final state interactions. I will then show recent more differential results using event shapes, underlying event estimators and correlations and discuss how these measurements can resolve the question of the underlying physics mechanism.

The ATLAS ITk Strip Detector for the High-Luminosity LHC

Author: Craig Wiglesworth, *Niels Bohr Institute*

The ATLAS Experiment is currently preparing a series of upgrades in preparation for the High-Luminosity LHC, due to start in 2027. One such upgrade will be to the inner tracking system which will be completely replaced with a brand new, all-silicon Inner Tracker, consisting of a pixel detector

near to the beam-line surrounded by a large-area strip tracking detector. This talk will present the status of the strip tracking system as the project moves into it's pre-production phase. The role of the Niels Bohr Institute within the project and the plans for the forthcoming production phase will be discussed.

PLENARY: 10 things you can do to improve your teaching and to make students learn more

Author: Ole Bjælde, Århus University

Do you also feel that the corona-period has made teaching more passive and less fun? Do you sometimes experience that it can be challenging to share your passion for physics and astronomy? And do you find it hard to figure out how much your students really learn? Here I will provide inspiration to 10 things you can do in your own teaching to make the teaching more exciting and to make your students learn more.

Warning: Do not read below this if you prefer to be surprised in the presentation

1. Activate prior knowledge
2. (Re)use digital solutions
3. Active learning!
4. Wait just ten seconds
5. Use continuous assessment
6. Use feedback loops
7. Let students give each other peer feedback
8. Less is more
9. Surprise your students
10. Let your students be innovative

SESSION: Computational Physics

Universalities in supercooled liquids: Relaxation, rheology, and crystallization

Author: Trond Sylvan Ingebrigtsen, *Roskilde University*

Supercooled liquids approaching the glass transition exhibit many common features such as a strong non-Arrhenius temperature dependence of their transport coefficients, growing dynamic heterogeneous regions, and more. This talk considers universal observations for supercooled liquids related to their relaxation, rheology, and crystallization pathway uncovered in past research. More specifically, we found: 1) A good description of the transport coefficients of supercooled binary mixtures via the excess entropy [1]. 2) A universal curve for nonlinear shear thinning via the excess entropy [2]. 3) An overlooked crystallization mechanism for supercooled mixtures relevant to, e.g., metallic glasses [3]. We connect these observations to relevant theories.

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Excited state dynamics simulations of an iron complex with strong solvation effects

Authors: Diana Bregenholt Zederkof¹; Sebastian Mai²; Kristoffer Haldrup¹; Leticia González²

¹ *DTU Physics*

² *University of Vienna*

The hunt for iron complexes with long-lived (ps) metal-to-ligand-charge-transfer (MLCT) excited states have gained recent interest among scientist due to their potential use as cheaper photosensitizers for e.g. solar energy harvesting [1, 2]. A model system for studying solvation related to MLCT states is the $[\text{Fe}(\text{CN})_4(\text{bpy})]^{2-}$ (bpy=2,2'-bipyridine) system. From an experimental point of view, the iron complex has shown a strong solvatochromic effect on the steady state absorption spectra [3] and excited state lifetimes [4], in particular related to MLCT states. To further investigate the ultrafast solvent effects, we carried out non-adiabatic dynamics simulations within the Surface Hopping including ARbitrary Couplings (SHARC) [5] formalism of the iron complex in water. Our studies examined the coupled electronic, structural and solvent dynamics of the $[\text{Fe}(\text{CN})_4(\text{bpy})]^{2-}$ complex in explicit solvent within 700 fs of excitation. Our simulations show that implicit solvation does not reproduce the experimental absorption spectrum, whereas the use of

explicit water solvation is in good agreement with experiments. We present time-dependent electronic populations, and extracted time constants of intersystem crossing, that is highly dependent on nuclear motion. Furthermore, we find a very different solvation structure around the bipyridine and the cyanide ligands, with the latter showing a strong bond to the nearest water solvent. We have simulated the solvent response and directly follow the reorganizing solvent within the earliest times after photoexcitation, in terms of time-dependent (angular-) radial distribution functions. To enhance the connection to experimental observations, we also simulated time-resolved wide-angle X-ray scattering (TR-WAXS) signals originating from both the solute-solute, solvent-solvent and the solute-solvent cross-term interactions.

Entropy Determination of an Atomic System via Data Compression

Author: Ian Douglass, *Roskilde University*

Co-author: Jeppe Dyre, *Roskilde University*

Determining the entropy of a chemical system is a long-standing problem in chemical physics. It can be used to determine a range of properties - including phase stability, optimal folded protein states, and thermodynamic quantities - but is computationally (and experimentally) quite difficult to calculate, and generally can only be found for equilibrium states. Recently however, it has been shown that an information theory approach can be used to qualitatively show phase transitions other non-equilibrium events using only position data and modern data compression methods. We present an extension to this, showing that equilibrium entropies of an atomic system can be quantitatively determined in the same manner, and that this method outperforms previous attempts to use structural data to calculate the entropy of a system.

GPU computing for physicists. (Use of OpenACC in McStas 3.0)

Author: Peter Willendrup¹

Co-authors: Emmanuel FARHI ²; Erik Bergbäck Knudsen ³; Mads Bertelsen ⁴; Torben Nielsen ⁵

¹ *Physics Department, Technical University of Denmark* ² *ILL*

³ *DTU Fysik* ⁴ *European Spallation Source* ⁵ *ESS-DMSC*

In recent years a number of high-level, easy to use programming tools for GPU acceleration have become available, providing an easier route to fast computing without the need of very deep and detailed understanding of the GPU hardware.

The presentation will describe one such high-level tool, namely the OpenACC precompiler-driven approach, and demonstrate how it was recently used to port the danish neutron Monte Carlo ray-tracer McStas to NVIDIA GPUs. The McStas package is widely used within the field of neutron-

scattering and applied e.g. to the design of scattering-instruments the ESS facility under construction in Lund, Sweden.

The presentation will demonstrate how specific simulation use-cases achieved a speedup exceeding 2 orders of magnitude with very limited change of code between CPU and GPU variants of the simulation.

SESSION: Condensed Phase Physics I

Manipulating magnetoelectrical materials

Author: Rasmus Toft-Petersen

Magnetoelectric materials are hosts to a coupling between electric polarization and magnetization, which is essentially caused by the intricacies of the quantum mechanical exchange interaction between the magnetic ions, which is incidentally also responsible for fridge magnets. Due to the possibility of using electrical fields to quickly switch between complex magnetic states, magnetoelectric materials are at the heart of some fascinating new proposals for improvements in IT-technology. Here, I will discuss how to manipulate this link between electrical polarization and magnetization. By mixing magnetic ions with different anisotropy in the right ratio, one can change the low temperature magnetic ground state of the material, that determines how the magnetoelectric effect works. The increased disorder gives rise to much larger polarization, and the new ground state changes the nature of the coupling. Using neutron scattering, we have determined the magnetic structure, and the electrical polarization is measured via the pyroelectric current. By means of Monte Carlo simulations, we have investigated the necessary conditions to fulfill in order to gain this control of magnetoelectric couplings. Surprisingly, the requirements are not strict, and current theoretical tools may be sufficient to probe the many options out there, without time consuming sample synthesis.

Van der Waals materials for spintronics and quantum technologies

Author: Yong Chen, *Århus University*

Van der Waals (vdW) or “two-dimensional” (2D) materials offer versatile building blocks and unprecedented opportunities to design and make new materials and heterostructures with diverse functionalities. They promise wide applications in energy-efficient and high performance

information processing, ranging from “spintronics” to various quantum technologies (quantum computing, quantum communication and quantum sensing). I will give an overview of various 2D/vdW materials and associated devices we make and study in my lab motivated by such applications. Examples include: vdW magnets and topological insulators (TIs) for spintronics devices; TI and hexagonal-boron-nitride (h-BN) based Josephson junctions that could improve superconducting qubits for quantum computing; defect centers or quantum emitters (single photon sources) in h-BN and transition metal dichalcogenides (TMDCs) for quantum communication and quantum sensing applications. We welcome new students and researchers to join our new lab in Aarhus University, Laboratory for Quantum Materials and Quantum Measurements, and Villum Center for Hybrid Quantum Materials and Devices, to further develop state of the art and new techniques to make, manipulate, and measure 2D/vdW materials and hybrid structures for new, emerging applications.

An improved cooling setup for clouds of cold Yb atoms

Author: Mogens From

Ultra-cold atomic clouds provide a well-known platform for Quantum Optics experiments, although one of the current limitations of the experimental platform are the achievable temperatures, densities, and loading rate of the clouds. This project explores new experimental methods for preparing clouds of cold Ytterbium atoms, specifically to provide a platform for modern experiments on atom-light interactions. We implement a modern Sawtooth Wave Adiabatic Passage cooling technique to obtain higher atom densities, using the narrow intercombination transition line in Yb. Furthermore, a setup is developed that can split and merge atomic clouds in optical dipole traps.

SESSION: Condensed Phase Physics II

Structure-activity relationships of catalytic materials with machine learning

Author: Mie Andersen, Aarhus Institute of Advanced Studies, Aarhus University

Materials with a catalytic function may be found in such diverse places as chemical reactors or as dust grains in molecular clouds in the interstellar space. Despite their crucial role in society and the Universe for accelerating chemical reactions, the reliable description of catalytic properties and the prediction of what materials may be even better catalysts than those we know already is still challenging. While it is possible to use electronic structure calculations (density functional theory,

DFT) to study simple reactions and simple model catalysts such as high-index facets of metals or oxides, the computational demands of such an approach can quickly become prohibitively large for realistic materials. Here I will present some of our recent work focused on developing machine learning models for understanding the relationship between structure, composition and catalytic activity and for identifying cheap and accurate descriptive models enabling high-throughput screening of catalytic materials.

Terahertz spectroscopy of solar cell materials: mobility, conductivity and functionality.

Author: Pernille Klarskov

Co-authors: Md. Tasnim Munshi ; Line Madsen ; Michel Hardenberg

Light carrying frequencies in the terahertz range has been widely used to study carrier dynamics in semiconductors since the plasma frequencies of these mostly fall within the terahertz range. Using proper models based on Drude theory, the plasma frequency can be exchanged for information such as the electron mobility, DC conductivity, sheet conductance, etc. Extracting such material parameters in an all-optical measurement i.e. without direct contact to the material is highly desired in fields such as electrical engineering or materials engineering, where optimum electrical properties are crucial.

In this presentation, we show two examples of different solar cell materials studied with terahertz spectroscopy. The first sample represents a plasmonic solar cell system where we study gold nanorods on a semiconductor surface with terahertz emission spectroscopy. This method is sensitive to the carrier mobility in the semiconductor substrate, which is enhanced with the increased coverage of gold nanorods on the surface. The second sample consists of a 100 nm thick TiO₂ film on a semiconductor substrate representing a charge extraction layer in organic solar cells. With terahertz time-domain spectroscopy we can extract the complex conductivity from the film discriminated from the substrate, and study the impact of thickness variations, surface morphology, oxidation, etc.

Hidden Scale Invariance in Liquid Crystal of Gay-Berne Fluids

Authors: Saeed Mehri; Jeppe Dyre; Trond Sylvan Ingebrigtsen, *Roskilde University*

Isomorphs are curves of invariant structure and dynamics in the thermodynamic phase diagram. They occur in systems with strong correlations between the constant-volume canonical-ensemble equilibrium fluctuations of potential energy and virial, which characterize the so-called R-simple (strongly correlating) systems. The Pearson correlation coefficient R between the thermal

equilibrium fluctuations of potential energy U and virial W is given by (where sharp brackets denote NVT canonical averages, and Δ denotes the deviation from equilibrium mean value):

$$R = \frac{\langle \Delta W \Delta U \rangle}{\sqrt{\langle (\Delta W)^2 \rangle \langle (\Delta U)^2 \rangle}}.$$

For an inverse power-law (IPL) system with pair potential proportional to r^{-n} in which r is the pair distance, the correlation is perfect, $R = 1$, because $W = (n/3)U$ for all microconfigurations. Somewhat smaller correlations still lead to fairly invariant structure and dynamics, and the class of R -simple liquids is defined by $R > 0.9$. It is important to note that isomorph invariances refer to structure and dynamics reported in the so-called reduced units. Isomorph theory has been applied to different classes of systems, including simple atomic systems in both liquid and solid phases, molecular systems, 10-bead Lennard-Jones chain, ionic liquids and metallic glasses.

Here in this study we applied the isomorph theory on a more complicated class of system; liquid crystals (LC) which composed of non-spherical molecules. This shape anisotropy allows them to exhibit a rich variety of structural phases as density and temperature are changed. Due to orientational and positional degrees of freedom these fluids exhibit phenomena not present in fluids of spherical particles. LCs are used in many applications and with different purposes, going from the well known display technologies to medical devices in biological systems.

A standard way to study LCs with computer simulation is using the Gay-Berne potential interaction which can describe mesophases in fluids of non-spherical particles. GB model gives us the flexibility to describe long ellipsoids, passing through spheres and ending in discotic particles, using one site per particle. This potential depends on four parameters, usually denoted as $GB(\kappa, \kappa', \mu, \nu)$, which are closely related to the shape of particles and the strength interaction between them. From all possible sets of parameters the most studied is the GB(3,5,2,1) fluids for ellipsoids, whose phase diagram, second rank orientational order parameter and pair distribution functions are already known. Our results show that the structure and dynamics of GB(3,5,2,1) fluids in the nematic and isotropic phase with $R > 0.9$ are invariant.

SESSION: Nuclear and Particle Physics (NICE II)

Exploring the evolution of the Early Universe at the first moment

Author: Anna Boye

Co-authors: Sarah Maj Schultz; Emil Emanuelsen Fischer; You Zhou, *Niels Bohr Institute, University of Copenhagen*

To increase our understanding of the evolution of the early universe, we studied the properties of the matter present at the time, Quark-Gluon-plasma (QGP), via anisotropic flow. Anisotropic flow is a key phenomenon that is sensitive to the properties of the QGP. By recreating the conditions present one microsecond after the big bang at the ALICE experiment, QGP is created for a short period of time after which it forms into hadrons that we can detect. In this talk, I will present the measurements of anisotropic flow in Pb-Pb collisions at 5.02 TeV, using the latest data taken at LHC Run 2. In addition, I will discuss the measurements in comparison to theoretical hydrodynamics calculations. This allows us to determine the viscosity of QGP as a perfect fluid as well as discuss the temperature dependency of the shear-viscosity-to-entropy-density-ratio of QGP.

Anisotropic flow in small collision systems

Author: Zuzana Moravcová, *NBI, Copenhagen*

Quark-gluon plasma (QGP) is a strongly interacting matter that existed shortly after the Big Bang and that can be produced in ultrarelativistic heavy-ion collisions at the Large Hadron Collider in CERN. One of the ways how to study its initial conditions and dynamic evolution is by measuring anisotropic flow. In recent years, several similar features have been observed in high multiplicity collisions of small colliding systems, such as proton-proton or proton-lead, nevertheless, it is yet unknown what is the origin of the observed final-state anisotropy – alongside the presence of a droplet of the quark-gluon plasma, another possible explanation can be the gluon saturation explained by the color glass condensate theory. In this talk, an experimental overview of anisotropic flow measured using multi-particle correlations in small collision systems will be presented together with comparisons to various hydrodynamic models.

The ATLAS Hardware Track Trigger for High Luminosity LHC

Author: Alessandra Camplani, *Niels Bohr Institute, University of Copenhagen*

The High-Luminosity upgrade of the Large Hadron Collider is scheduled to begin in 2026 and will lead to a number of collisions ten times higher in the ATLAS experiment. To cope with this increase, ATLAS is preparing a series of upgrades including the installation of new detectors using state-of-the-art technology, the replacement of ageing electronics, and the upgrade of its Trigger and Data Acquisition (TDAQ) system.

This talk focuses on the TDAQ upgrade and in particular on the Hardware-based Track Trigger (HTT) system. The HTT is a new massively parallel system, based on Field Programmable Gate Arrays

(FPGAs) for fast data processing and custom Associative Memories (AM) ASICs performing pattern recognition. The goal of the HTT project is to perform very fast reconstruction of particle tracks, faster than what could be done in software. HTT is a co-processor that complements the ATLAS CPU-based processing farm.

Improved e/photon energy reconstruction at ATLAS using a CNN

Authors: Malte AlgrenNone; Troels Petersen, *Niels Bohr Institute*

The e/photon energy resolution is a key parameter of both the EM calorimeter and several Higgs analyses, most notably the di-photon final state. We present an improvement in the precision of the energy regression for electrons and photons, based on a convolution neural network (CNN) architecture. The algorithm has been designed to predict the energy of electrons and photons in channels Zee (for control) and Hyy (main target). This has proven to be effective with an improved energy resolution of roughly 16–20% in both Monte Carlo and (Zee) data.

We have also succeeded in training directly in data, avoiding misalignment between MC and data. An additional advantage is the ability to obtain reliable uncertainties on the predicted energies by changing loss function. This can in turn be used to remove/reweight poorly reconstructed events.

PLENARY: Increasing the complexity of quantum devices and their tuning

Authors: Anasua Chatterjee, *Niels Bohr Institute*

A hundred years since the heyday of Niels Bohr, quantum technology is maturing around the world. However, a large roadblock is the scalability of the underlying quantum hardware, which can involve hundreds to thousands of qubits. Currently, in all state-of-the-art research laboratories, quantum dots and qubits are painstakingly tuned by hand, one by one, a process which must be repeated incessantly due to environmental drift. As device complexity grows, even for small processors and especially for gate-voltage-tuned processors, tuning the system becomes prohibitively expensive. Also, the volume of data generated by simple gate-voltage sweeps becomes unmanageably large and complex, beyond the level at which humans can intuitively process and take action on the patterns underlying it. In this talk, I will describe our efforts to use another nascent yet powerful technology, machine learning, to automate the process of tuning, optimization and operation of quantum technology.

PLENARY: The modelling of Covid-19... physics thinking during an epidemic

Author: Troels Christian Petersen

With the outbreak of Covid-19 in Denmark, the government was in sudden need of more people, who could quickly analyze data and model the epidemic, since this was greatly needed for planning and decision making. Among the expert team of Statens Serum Institute (SSI) were several physicists, knowing nothing about epidemiology, but a lot about data and models.

I will - being part of this SSI team - try to give an insight into the dynamics of the epidemic, and also the tools for modelling/fitting/estimating the effects. Many things follow's a physicists line of thinking, also including (large) uncertainties and "impossible" measurements. The largest deviation from physics is the unpredictability of human behavior, but even this has certain elements of feedback systems in it.

Tuesday

PLENARY: How to make Computing (& Physics?) more Appealing to Women, Recruitment & Retention Perspective.

Author: Claus Brabrand, *Head of Center for Computing Education Research (CCER), IT University of Copenhagen (ITU).*

In 2015, the ratio of women on the Bachelor of Software Development (BSWU) at the IT University of Copenhagen (ITU) was one in ten (10%). ITU decided to do something about this and implemented a number of interventions aimed at increasing diversity; in particular, the number of women. In 2020, the ratio of women on BSWU had risen to almost one in four (23%). This talk will present key insights from ITU's efforts to recruit and retain more women in Computing. We will also look at how to make educational activities more appealing to women; modifying the themes (scenarios) of exercises/projects/examples, dramatically impacts their appeal to women. This is based on two recent experiments involving around 500 high-school students (recruitment perspective) and about 150 university students (retention perspective). We will also speculate on how to transfer the ideas from the context of Computer Science to Physics.

SESSION: Education and science communication

The Mars Base Project: Investigating a grand narrative approach to physics teaching with network analysis

Authors: Jesper Bruun; Viktor Holm; Karen Alavi Voigt, *KU, Science, Institut for Naturfagenes Didaktik*

In this talk, we show how The Mars Base Project uses a scenario based learning game to develop materials for teaching high-school physics. Furthermore, we briefly show, how we use network analysis to investigate how, why and what students learn using this approach. Our live illustration of the learning game will involve possible active participation by the audience. Here we will illustrate how teaching with The Mars Base takes involves an interactive and partly digital story set in the future, where students take on the role of pioneers on Mars. After the live presentation, we will briefly discuss the methods we use to collect and analyze educational data. We are currently investigating how to use both manual and machine learning techniques in conjunction with network analysis to convert audio and video to data we can analyze quantitatively and qualitatively.

Ill-structured problems fostering curiosity, creativity, and critical thinking in astronomy

Author: Lenka Otap

Ill-structured problems can be used to foster curiosity, creativity, and critical thinking in higher education. An example of an exercise for high school astronomy, Exoplanet Design, combining science and creativity using ill-structured problem-based learning, tested with a high school class in an online classroom. How did the students solve the exercise and what were the results?

Experimental physics at the Niels Bohr Institute

Author: Athene Demuth, *Niels Bohr Institute*

Experimental physics is an essential part of studying physics at the Niels Bohr Institute. In my presentation, I will show how we teach experimental physics and bring in my own experience and fascination with the field. Both as a student and as a teaching assistant, I enjoy being in a laboratory and to get a hands-on experience with the theory and formulas that we learn. It is there, in the laboratory, that I learn how we can perceive and analyse the world with the physicist's approach, and how one can collect data and use it to put our surroundings into numbers and to test our theoretical predictions. I am very fond of the way that we handle experimental physics at NBI and in my presentation I will present some of our teaching methods and illustrate with some of our experiments.

Ellære i gymnasiet med Arduino

Author: Jens Krog, *Bagsværd Kostskole og Gymnasium*

Sensorer er for nyligt blevet tilføjet til kernestoffet i fysikfaget på de gymnasiale uddannelser, hvilket kræver indførelsen af nye eksperimentelle forløb. I disse eksperimenter er mikrocontrolleren fra Arduino et oplagt redskab, fordi den giver mulighed for at undersøge en lang række sensorer med relativt simpelt og billigt udstyr. Desværre er indlæringskurven for brugen af en mikrocontroller stejl, hvilket kan komplicere elevernes oplevelse af selve sensorene unødigt. Vi foreslår derfor en række forsøg som giver mulighed for at stifte bekendtskab med Arduinoen allerede i begyndelsen af forløbet om ellære. Forsøgene strækker sig fra den simpleste begrebsdannelse vedrørende elektriske kredsløb og til databehandling og styring af simple kredsløb gennem små programmer, som køres på mikrocontrolleren. Forhåbningen er at når eleverne undervises i fundamental ellære gennem brugen af en mikrocontroller, så vil de have betydeligt lettere adgang til eksperimentelt arbejde med sensorer.

SESSION: Nuclear and Particle Physics (NICE III)

Challenging the lepton sector of the standard model

Author: stefania xella, *hep*

Lepton flavour conservation and lepton universality are assumed in our description of particle processes at the fundamental level. Recent collider results indicate that experimental precision now allows to challenge such assumptions, and first deviations appear in the data. this calls for questions: which new physics can explain breaking of such assumptions? which searches should we further focus on? I summarise my research interest and activity in this area.

A Graph Neural Network Approach to Low Energy Event Reconstruction in IceCube Neutrino Observatory

Author: Rasmus Ørsøe, *NBI*

This work investigates a graph neural network (GNN) approach to low energy event reconstruction in IceCube Neutrino Observatory by treating level7 oscNext samples as point cloud graph representations of low energy neutrino events. A GNN model is proposed and tested against current low energy reconstruction methods in both classification and regression tasks in MC data and on IC86.11 measurements. In MC data, this work finds a 15% increase in neutrino signal as compared to the current final level7 neutrino classifier, or equivalently, a reduction of background by 80% at the same neutrino signal strength. In addition, this work records 11.7%, 22.4% and 16.3% improvement in the widths of error distributions for regression targets *azimuth*, *energy_log10* and *zenith*, respectively, as compared to RetroReco in the neutrino oscillation relevant energy range of 0 to 1.5 \log_{10} GeV. The proposed model is capable of producing reconstructions at speeds of 15.000 events pr. second as compared to 5 - 40 seconds pr. event for RetroReco, which opens the potential for cosmic alerts from low energy neutrinos. Lastly, this work contains a characterization of at least part of the current pulse noise in IceCube Upgrade MC data, and finds these to originate from suspicious same-pmt activation patterns from mDOMs.

Simulations of the FoCal upgrade for ALICE

Author: Sarah Andersson, *HEHI NBI*

This project focuses on simulating the hadronic part of the proposed forward electromagnetic and hadronic calorimeter (FoCal) for ALICE to be installed at LHC CERN.

Idealized simulations have been build in ROOT, using the GEANT simulation tool kit, creating a hadronic calorimeter module consisting of $25 \cdot 25$ capillary tubes and a test beam of π^- . The simulations have been build as to make sure they are easily adjustable, and made to constitute a good baseline for further development of simulations of the full Focal detector. This study has tested the influence of a randomized incident angle θ of the test beam, the geometry of the capillary tubes, the ratio of absorber to scintillator material and the effect of a simplified electromagnetic calorimeter in front of Hcal. This resulted in 5 different simulations for the circular and hexagonal shape, respectively. These simulations have been analyzed based on energy distribution pr. primary particle, distribution along the longitudinal direction of the calorimeter, the compensation criteria: $\frac{e}{h} = 1$ and others.

This study yielded results implying a favorable ratio of absorber to scintillator of 3 to 1, based on the energy resolution from computed fits of the energy deposition and an analysis of the calorimeter signal split up into a hadronic and electromagnetic part. This study also implied that the EM part of the signal is the primary source of the Landau tail in the energy resolution, and that the geometry with hexagonal pipes (no air gaps), yields a better proportionality between incident energy and deposited energy.

Nuclear deformation in Pb-Pb and Xe-Xe collisions

Author: Emil Gorm Nielsen, *University of Copenhagen (DK)*

The quadrupole deformation of heavy nuclei is not directly accessible experimentally and rely on theoretical predictions in order to extract numerical values. The nuclear structure has traditionally been studied with low-energy experiments, however, ultrarelativistic heavy-ion collisions may serve as an alternative probe of the quadrupole deformation parameter β_2 , through the correlations between the anisotropic flow v_n and the average transverse momentum $[p_T]$. The anisotropic flow is sensitive to the shape of the initial overlap between the colliding nuclei, while the average transverse momentum is sensitive to the size of the initial system. By studying the correlation between different v_n and $[p_T]$, information about the quadrupole deformation of different colliding nuclear species can be inferred. In addition, this observable can give additional constraints on initial conditions of the quark-gluon plasma created in the collisions. The correlations are studied at different centralities of Xe-Xe collisions at $\sqrt{s_{NN}} = 5.44$ TeV and Pb-Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV, with the Pb-Pb collisions serving as a baseline for the study of the deformation of the Xe nuclei.

PLENARY: Gastronomy Unravelling by Physics

Author: Mathias P. Clausen, *SDU Biotechnology*

Gastrophysics has emerged as a new scientific discipline in which a physical methodology is applied to tackle questions of gastronomic origin. The scientific questions are motivated by various elements from the preparation of food as well as the process of eating. Gastronomic phenomena are studied using theoretical, experimental, and computational approaches across length scales from sub-molecular to entire foods in order to provide a fundamental understanding of the system of interest.

The presentation will introduce gastrophysics as a scientific field and provide historical examples showcasing how physics has enabled the advancement of cooking and gastronomy, and vice versa, how gastronomic reflections has led to new physical insight.

Further, the presentation will include recent studies focusing on textural aspects of food and the relation between the microscopic structure of food materials studied with various optical microscopy methods (e.g. CARS microscopy and super-resolution STED microscopy) and their macroscopic textural behaviour and mouthfeel. Presented studies includes investigations of protein network formation during temperature controlled cooking (sous vide) of egg, lipid droplet characterisation in foie gras emulsions, and molecular redistribution in gastronomic preparations of jellyfish that transforms the soft gel to a crunchy texture, and where the application of gel-theory has enabled the preparation of jellyfish crisps.

Posters

Geophysical modeling with Veros

Authors: Dion Häfner; Markus Jochum; Marta Mrozowska; Roman Nuterman, University of Copenhagen (UCPH)

Modern geophysics and climate science rely heavily on numerical models. A plethora of these exists in the community, however the majority of them are written in C or Fortran, which can be difficult to approach by beginners. We present an answer to this: Veros, the versatile ocean simulator. Veros is a full-fledged, high performance ocean model written in pure Python. Thanks to this, Veros is easy to run and modify, which creates not only a powerful tool for scientific research, but also an effective teaching resource. We present 2 case studies which demonstrate how Veros can be used to familiarize students with programming in Python, geophysical modeling and ocean dynamics.

A Scattering equation builder

Author: Tobias Jarrett

Neutron and small-angle X-ray scattering are ideal techniques to characterize molecular structure and self-assembly at the nano scale. The resulting spectra require extensive modelling to infer the structure. For example could be linear or branched polymer structure in solution. My poster presents a formalism [Svaneborg, C., & Pedersen, J. S. (2012). A Formalism for Scattering of Complex Composite Structures: I Applications to Branched Structures of Asymmetric Sub-Units. *Virtual Journal of Biological Physics Research*, 23(6).] to derive the form factor of such composite structures and its implementation in C++. The formalism is similar to Feynman diagrams, where one can represent an equation in the form of a diagram. The implementation allows expressions for form factors to be derived symbolically for model structures composed of known sub-units e.g. random walk polymers and rigid sticks. We hope the ability to rapidly and cheaply define structural models and automatically derive expressions for its small-angle scattering spectrum will facilitate and accelerate analysis of experimental data.

Magnetic heating of nanoparticles

Authors: Bianca Hansen; Lise Hanson

Co-authors: Cathrine Frandsen ; Niels Bech Christensen, *Danmarks Tekniske Universitet*

Magnetic hyperthermia is a promising technique in cancer treatment for killing or weakening the cancer cells by exposing injected magnetic nanoparticles to an external alternating magnetic field.

For the development of hyperthermia, it is vital to be capable of comparing the heating properties of different magnetic nanoparticles. However, big discrepancies are present across different laboratories when measuring on the same type of magnetic nanoparticles. This provides a need to find the potential sources of systematic errors and to obtain a consensus on how to perform measurements and data treatment.

We present our investigation of determining potential systematic errors and our suggestions to improving the accuracy of the measurements. Our results suggest that the commonly applied heat transfer model is too simple in experiments where a nanoparticle sample is surrounded by insulation material. This investigation has shown that the environment has a strong impact on the measured heating properties which is rarely considered in literature.

Classical Radiation Reaction

Author: Christian Nielsen, *Aarhus Universitet*

The classical equation of motion for a charged particle moving in an electromagnetic field is usually described through Lorentz force, which predicts that a particle moving perpendicular to a static magnetic field would continue on a circular trajectory indefinitely. In reality this is not true, when charged particles accelerate they emit radiation, causing the orbit of the particle to spiral inwards until all its energy has been emitted. This is the century old problem of radiation reaction, which theoretically have been solved decades ago by adding a dampening force on the equation of motion, giving what we call the Landau-Lifshitz equation of motion. In this project, for the first time, we investigate the applicability of the Landau-Lifshitz equation experimentally at the CERN SPS H4 beamline. When impinging 40-80 GeV electrons on to oriented diamond single crystals, these electrons experience incredibly strong electromagnetic fields in their rest frame, causing them to emit radiation comparable to their initial energy. Since the emitted radiation is coupled directly to the trajectory of the electrons inside the crystal, we can compare the experimental photon spectra with simulated photon spectra using either the Landau-Lifshitz equation or just the Lorentz equation without radiation reaction. We found that the radiation spectra calculated using the Landau-Lifshitz equation was in remarkable agreement with the experimental spectra, when including simple quantum corrections to the emission process and the radiation intensity, while the Lorentz force was inadequate in describing the experimental data.

From superconducting circuits to quantum technology

Author: Stig Elkjær Rasmussen, *Aarhus University*

Quantum information processing is a rapidly emerging field within physics. Universities and large tech companies, such as Google, IBM, and Microsoft are racing towards quantum supremacy, i.e.,

performing calculations on a quantum processor more efficiently than possible on a classical processor.

A particularly promising platform for such scalable quantum technology is superconducting circuits used for implementing quantum bits (qubits). In this project we consider how to make qubits from such superconducting circuits and how one should operate on these qubits such that they can be used for actual calculations.

Superconducting qubits are made from macroscopic components: capacitor, inductors, and superconducting Josephson junctions. These can be put together in electrical circuit in order to create an anharmonic oscillator, which can be truncated into the lowest levels, effectively creating a qubit. These qubit can be controlled using microwave driving in order to create single-qubit gates and coupled in order to perform two-qubit gates. By performing such gates on an array of qubits it is possible to perform algorithms on the qubits. These quantum algorithm span from contemporary hybrid quantum classical algorithm, such as the variational quantum eigensolver or the quantum approximate optimization algorithm, to futuristic full quantum machine learning, such as quantum generative adversarial networks.

High statistics study of ^{12}B beta-decay

Author: Andreas Gad, *Department of Physics and Astronomy, Aarhus University*

The triple- α reaction is paramount for understanding the abundance of ^{12}C and ^{16}O in the universe. The reaction happens mainly through the famous Hoyle state in ^{12}C , but the low energy tails of higher lying 0^+ and 2^+ states will also contribute. The region from 8-12 MeV excitation energy in ^{12}C is dominated by a broad continuum, and it is therefore difficult to extract precise parameters for these levels.

The experiment I257 done at IGISOL, Jyväskylä, is a high statistics experiment measuring the β -delayed 3α -decay of ^{12}B . We measure the full kinematics of the three outgoing α -particles using six Double sided Silicon Strip Detectors (DSSD's) and 5 Single sided Silicon Detectors (SSD's), placed in a compact cube resulting in a large solid angle coverage of 50%. The full-kinematics measurement allows us to study the decay mechanisms in greater detail than previously possible.

The spectra are analyzed using R-matrix theory to determine the properties of the levels.

Tailoring superconducting circuits for surface codes

Author: Kasper Sangild Christensen, *Aarhus University - IFA*

Quantum computers has the potential to spectacularly outperform classical computers in certain types of problems. By utilizing the quantum phenomena of superposition and entanglement, novel

algorithms have been design that have no classical counterpart. Perhaps most famously Shor's algorithm is capable of prime factorization much faster than any known classical algorithm. However, it may be a long time before a large scale quantum computer capable of solving actual interesting problems faster than any classical supercomputer is realized. Quantum systems are susceptible to noise which destroys the encoded quantum information, and the development of quantum error correction is therefore crucial. One of the most promising avenues for realizing error correction are through surface codes. By placing many qubits on a lattice and running a surface code protocol, a single qubit worth of information can be protected. Surface codes requires measuring certain operators known as stabilizers. These are typically exotic many body observables that are difficult to measure on most platforms. This project aims to leverage the flexibility and design space of superconducting circuits to construct scalable systems where the stabilizers are easily measured.

AlphaPI I

Authors: Anders Sandermann Mortensen; Benjamin Karstensen, *Student at NBI*

In the course of the Alpha-Pi Project it has been investigated if a Raspberry Pi single board computer and PiCamera (Sony IMX219 8-megapixel) can be used to detect α -particles and measure their energy in a way that is suitable for educational purposes.

The counting abilities and energy measurement abilities of the pi-camera have been investigated. Exponential damping of radiation intensity and geometric dilution of alpha-particles have successfully been observed with the pi-camera. Thus, We would like to present the potential of the picamera as a new means of performing educational experiments.

The relation between measured intensity and particle energy is still in testing.

Approaching High-Frequency Rheology on Rubbers: Closing the Gap in Broadband Mechanical Spectroscopy

Authors: Mathias Mikkelsen¹; Jorge Lacayo-Pineda²; Tina Hecksher³

Co-authors: Niclas Lindemann ²; Ali Karimi ²; Tage Christensen ³

¹ *Glass and Time, Roskilde University, Denmark & Research and Development, Continental Reifen, Hannover, Germany*

² *Research and Development, Continental Reifen Deutschland GmbH, Hannover, Germany*

³ *Glass and Time, IMFUFA, Department of Science and Environment, Roskilde University, Roskilde, Denmark*

The dynamic mechanical properties of tread compounds at certain frequency ranges are used as predictors of the tyre performance: low frequencies determine the rolling resistance, while higher frequencies are most important for braking and wear.

Therefore, measuring these properties over a very broad range of frequencies is imperative for the optimization process. Standard equipment measures below 100 Hz and higher frequencies are extrapolated by invoking the so-called *time-temperature superposition* principle, which may lead to erroneous predictions, especially for the high frequency region. We therefore need broadband techniques which can probe all relevant frequencies directly.

We present such a broadband technique, developed from the *piezoelectric shear modulus gauge* which was originally developed and used at Roskilde University for fundamental research into viscous liquids. This enables us to probe the shear modulus of rubbers across several decades of frequencies – from mHz to tens of kHz.

Revisiting the Stokes-Einstein relation without a hydrodynamic diameter

Authors: Lorenzo Costigliola¹; David M. Heyes²; Thomas Schrøder³; Jeppe Dyre¹

¹ Roskilde University

² Imperial College London

³ Glas & Time, Roskilde University

We present diffusion coefficient and shear viscosity data for the Lennard-Jones fluid along nine isochores above the critical density, each involving a temperature variation of roughly two orders of magnitude. The data are analyzed with respect to the Stokes-Einstein (SE) relation, which exhibits a gradual breakdown at high temperatures. This is rationalized in terms of the fact that the reduced diffusion coefficient \tilde{D} and the reduced viscosity $\tilde{\eta}$ are both constant along the system's isomorphs.

It is shown that $\tilde{D}\tilde{\eta}$ is a function of $T/T_{Ref}(\rho)$ in which T is temperature, ρ is density, and $T_{Ref}(\rho)$ is the temperature along a reference isomorph. This allows one to successfully predict the viscosity from the diffusion coefficient throughout the studied region of the thermodynamic phase diagram, also for the state points at which SE does not apply. The viscosities calculated in this way are found to be in good agreement with the equation previously proposed by the same authors.

AlphaPi II

Authors: Benjamin Karstensen; Anders Sandermann Mortensen, *Student at NBI*

I will talk about the Raspberry Pi 4 SBC and accessories and how they were used in the AlphaPi project. I will also explain how we used python to write a code with which we currently can process about 17 fps reliably over the course of several hours. Finally, I present several ideas on how to improve the software with respect to processing power but also user friendliness.

Characterization of SiPM for the ALICE forward calorimeter

Author: Laura Marie Dufke, *Copenhagen University*

The inspiration behind this project is the ALICE collaborations proposal of adding a forward electromagnetic and hadronic calorimeter (FoCal) as an upgrade to the ALICE experiment.

In my studies, I have focused on the hadronic part of FoCal (FoCal-H), especially the Silicon Photomultipliers (SiPM), which will read out scintillating fibers.

According to their vendor reported performance and price, the SiPMs seems to be an ideal detector for reading out signals from the FoCal-H scintillators. In this project, I have subjected SiPMs from the vendors; Hamamatsu, Broadcom, AdvanSiD, and KETEK, to two sets of tests to determine which of them has optimum price to performance. The SiPMs performance parameters, which has been tested are; (1) Photon detection efficiency, by testing single photon events, and (2) Gain versus response, at maximum and minimum overvoltage.

The results of these test will be used to choose which SiPM should be used for the FoCal-H prototype, which will be constructed in the summer of 2021.

Simple Readout System for SiPM's

Author: Alexander Buhl, *Copenhagen University*

This project aims to develop a simple readout system for small (>20) numbers of SiPMs.

Such a readout system would, for example, allow for the construction of a position sensitive scintillator based trigger detectors.

The first question in the study was, what is the time resolution of SiPMs reading out a 1x1x20cm³ scintillator?

With sufficiently good time resolution, it would be possible to determine where along the scintillator a charged particle passed.

In my tests, however, the timing resolution (300 ps) was not sufficient to determine the position to better than 5cm.

Thus, I built and tested a system comprising two perpendicular layers each with 5 of the scintillators tested previously.

By finding coincidences between an individual scintillator in layer one with one in layer two, one can obtain a position sensitivity of 1 cm.

This design was tested using both radioactive sources and cosmic ray muons. Results will be reported in this contribution

Vikings in the Classroom

Author: philip miguel kofoed, Marie Kruse Skole (*gymnasie-afdelingen*)

In this poster-presentation some of the possibilities to include Vikings into the curriculum in high school physics will be presented. The major idea is to twist the classical experiments to give a greater storytelling and show that physics is a long-lasting discipline which we have used since the beginning of time. Vikings has recently been featuring in pop-culture with both Netflix, Vikings, the Danish European Song Contest 2018. Yet physics teachers seem slow to pick up these trends and incorporate those into our storytelling. As examples; the friction coefficient, the law of Archimedes and motion into dimensions.

From personal experience, I would claim that a lot of students only believes the laws of physics to exist within the walls of the physics classroom. With these experiments it will both be possible to advance with in the theory, as well as taking the students away from the classroom and out into the nature.

Structural dynamics of the ultrafast photodissociation of triiodide observed with time-resolved wide-angle X-ray scattering

Author: Amke Nimmrich

Co-authors: Matthijs Panman 1; Stephan Niebling 2; Oskar Berntsson 3; Elisa Biasin 4; Jonas Petersson 5; Maria Hoernke 6; Alexander Björling 3; Emil Gustavsson 7; Tim B. van Driel 8; Asmus O. Dohn 8; Mads Laursen 8; Diana B. Zederkof 8; Kensuke Tono 9; Tetsuo Katayama 9; Shigeki Owada 9; Martin M. Nielsen 8; Jan Davidsson 10; Jens Uhlig 5; Kristoffer Haldrup 8; Jochen S. Hub 11; Sebastian Westenhoff 1

1 *University of Gothenburg* 2 *University of Hamburg* 3 *MAX IV Laboratory* 4 *Stanford University, SLAC National Accelerator Laboratory* 5 *Lund University* 6 *University of Freiburg* 7 *Karolinska Institutet* 8 *Technical University of Denmark* 9 *RIKEN SPring-8 Center* 10 *Uppsala University* 11 *Saarland University*

Resolving the structural dynamics of fundamental reaction events is necessary for a deeper understanding of solution phase chemical reactions. Using X-ray scattering methods at Free Electron Lasers direct observation of the dynamics on fs timescales is made accessible.

Here, we investigate the photodissociation of triiodide in four solvents using femto- to nanosecond time-resolved wide-angle X-ray scattering (TRWAXS).

Upon absorption of 400 nm light triiodide in solution dissociates into diiodide and iodine fragments. This reaction involves several fundamental reaction steps, such as bond cleavage and solvent cage escape. Additionally, the scattering from the comparably electron-dense iodine atoms contrasts well against the solvent background making it the ideal system to investigate solution phase reactions with X-ray scattering.

Using TRWAXS, we resolve in real time the structural evolution of the bond cleavage, internal rearrangements, solvent-cage escape, and bond reformation after photoexcitation with 400 nm. Further, performing the experiment in different solvents showed how the reaction is influenced by the solvent environment. The data reveal a solvent dependency of the speed of the bond dissociation as well as of the cage escape probability.

The resolved structural dynamics present a comprehensive picture of the solvent influence on structure and dynamics of chemical reactions.

Classical spin liquid or extended criticality in a frustrated antiferromagnet

Author: Sofie Janas,*DTU*

Frustrated magnetism, in which competing exchange interactions suppress magnetic order, is a hot topic within condensed matter physics. One of the most heavily discussed topics is the quantum spin liquid (QSL), which is defined as a fluidlike state, where the magnetic spins are highly correlated but continue to fluctuate down to temperatures of absolute zero, although experimental verification is still contentious. Many frustrated compounds show features reminiscent of QSLs but order magnetically at finite temperatures, which excludes them as QSL candidates. Above this ordering these compounds are referred to as classical spin liquids, as cooperative paramagnets, or merely as having spin-liquid-like phases, although no clear definition of these terms is readily available. By using neutron spectroscopy on a classical triangular-lattice frustrated antiferromagnet, we investigate the classical spin liquid phase and its coexistence with order. We model the dynamics in the ordered and correlated disordered phase as critical spin correlations in a two-dimensional magnetic state, and propose that our findings may provide a general framework to understand features attributed to classical spin liquids.

IceCube Upgrade oscillation sensitivities

Authors: James Mead; Tom Stuttard,*Niels Bohr Institute, IceCube*

The IceCube Neutrino Observatory is a cubic-kilometre particle detector embedded within the Antarctic ice sheet. Neutrinos produced in Earth's atmosphere can pass through the planet and up through the instrumented ice. Over this distance, these neutrinos experience flavour oscillations, quantum mechanical effects which offer the only laboratory signal of physics beyond the Standard Model. By deploying seven additional columns of new sensors at ten times higher density than the rest of IceCube, the IceCube Upgrade is expected to provide world-leading sensitivity to neutrino

oscillations. This work presents up-to-date expectations for the IceCube Upgrade's oscillations precision measurements.

Top Quark Pair Production at a Future e^+e^- Collider

Author: Julie Torndal,*NBI*

The future of Particle Physics is looking to return to lepton colliders and move the limits on the precision frontier. FCC-ee is one of the proposed future e^+e^- colliders that can study particle properties at an unprecedented precision. This study aims to analyse top-quark electroweak couplings in pair produced events in order to gauge the sensitivity to anomalous couplings of the top quark to the photon and the Z boson at the FCC-ee at $\sqrt{s} = 365$ GeV. The study focuses on the semileptonic channel only with signal and background samples produced within the FCCSW package. The performance of a set of jet algorithms and recombination schemes are studied where the Durham algorithm with the E-scheme was chosen as the jet definition for this study. The event selection is presented which improves the significance on the signal to background ratio by a factor of ~ 8 .

Tau decay mode identification in a LAr electromagnetic calorimeter at FCC-ee

Author: Katinka Wandall

With the construction of the Future Circular Colliders (FCC) the LHC, today's most powerful accelerator ever build, will be exceeded in both size, energy and luminosity. One of the goals for FCC is gathering high precision measurements of key Standard Model parameters. In order to achieve this goal, it is vital to construct the best calorimeters and detectors possible and a liquid argon (LAr) electromagnetic calorimeter (ECAL) is one potential solution. This study investigates the performance of such an ECAL at the FCC-ee collider through identifications and separations of hadronic τ decay channels. A variant of a noble liquid ECAL has been implemented in the current ATLAS experiment at CERN and has proven to be highly stable and provide good energy measurements indicating fine prospects for these calorimeter types. However, the proposed calorimeter for the FCC-ee is a brand new design and therefore all particle identification and clustering methods must be implemented from scratch - a fundamental step for future analysis. This is done by first concentrating on single particle gun studies in the detector which can later be transferred to full τ decays in order to form and optimize the migration matrix of its hadronic decays. It is also intended to expand these studies to a liquid krypton electromagnetic calorimeter with the aim of comparing the performance of the two designs.

Preliminary study of the excited energy landscape of $[\text{Fe}(\text{bpy})(\text{CN})_4]^{2-}$

Author: Morten Haubro

Co-authors: Diana Bregenholt Zederkof; Kristoffer Haldrup, *DTU Physics*

Iron centered complexes have been the subject of extensive studies due to the prospect of using them in dye-sensitized solar cells, as a replacement for the more expensive and scarce Ruthenium and Iridium centered molecules. Making this substitution requires that the first excited state, the so called metal to ligand charge transfer (MLCT) state, is long lived. In general this is not the case for the iron centered complexes. $[\text{Fe}(\text{bpy})(\text{CN})_4]^{2-}$ is of particular interest because the excited energy landscape of the compound is highly tunable by changing the solvent. Using spectroscopy methods, other studies have found that the lifetime of the MLCT state ranges from ~ 20 ps in DMSO down to ~ 100 fs in water. Understanding this discrepancy would require an intimate understanding of the solvation dynamics associated with photo-exciting the system. We present an ultrafast x-ray study of $[\text{Fe}(\text{bpy})(\text{CN})_4]^{2-}$ in water from the Linac Coherent Light Source. The ultra short and extremely intense X-ray pulses available at an X-ray free electron laser enables resolution of the structural changes in the solvent as well as the solute immediately after photo excitation, with a time resolution down to ~ 100 fs. In this work we present a preliminary comparison between theoretical simulations done in the SHARC framework and experimental data.