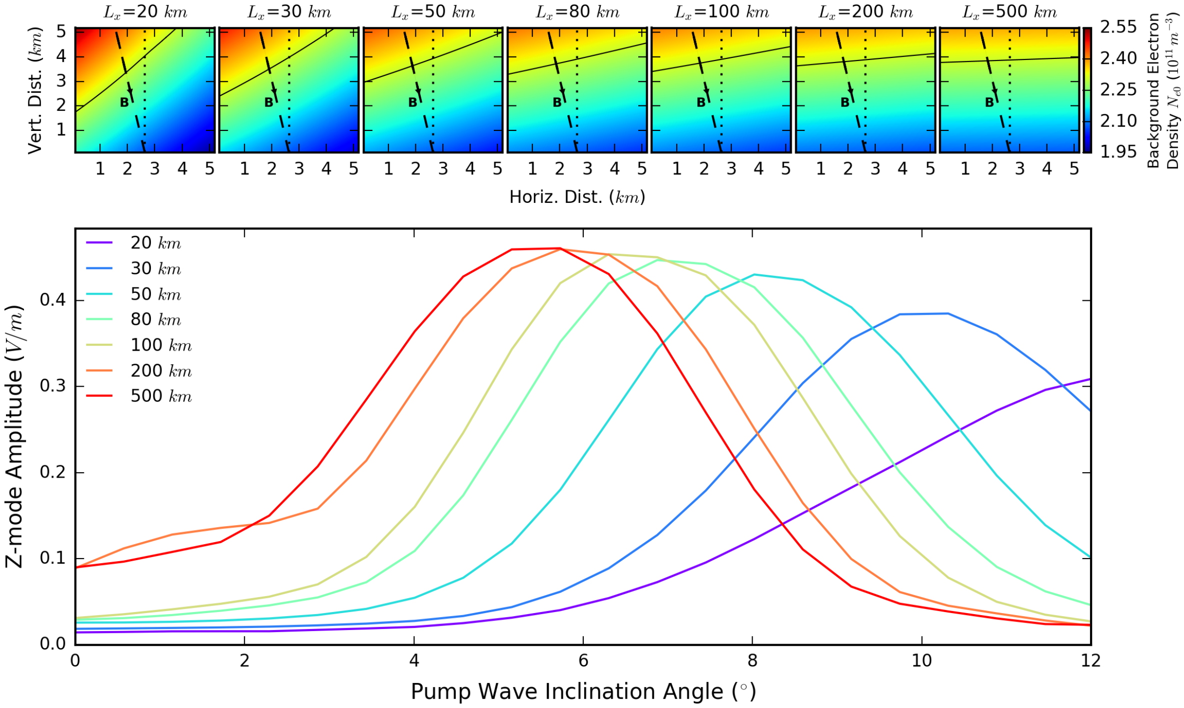
SUMMER 2017

IOP Institute of Physics
Computational Physics Group
Newsletter



Finite-Difference Time-Domain Simulations of EM Wave and Plasma Interactions in the Ionosphere
(image courtesy of Dr P. D. Cannon)

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This Newsletter...

Dear Readers,

The feature article for this bumper edition of the newsletter is an invited contribution by Dr P. D. Cannon from the Lancaster University, a runner-up of the 2016 IoP Computational Physics Group PhD Prize, on *'Finite-Difference Time-Domain Simulations of EM Wave and Plasma Interactions in the Ionosphere'*.
Dr P. D. Cannon also kindly provided the cover image for this edition.
In addition, we have a comprehensive report from the (QUPLA) Quantum Plasmonic workshop, the Euro-TMCS II: Theory, Modeling and computational Methods for Semiconductors and TYC-Toucan workshop on Shaping Nanocatalysts.

Most URLs in the newsletter have web hyperlinks and clicking on them should take you to the corresponding page. The current edition of the newsletter can be found online at:

`www.iop.org/activity/groups/subject/comp/news/page_40572.html`

with previous editions at:

`www.iop.org/activity/groups/subject/comp/news/archive/page_53142.html`

As always, we value your feedback and suggestions. Enjoy this edition!

Marco Pinna, Newsletter Editor ✉ mpinna@lincoln.ac.uk

(on behalf of the The Computational Physics Group Committee).

Finite-Difference Time-Domain Simulations of EM Wave and Plasma Interactions in the Ionosphere

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Abstract

Ionospheric modification by means of high-power electromagnetic (EM) waves can result in the excitation of a diverse range of plasma waves and instabilities. In this article we summarise of the development and application of a GPU-accelerated finite-difference time-domain (FDTD) code designed to simulate the time-explicit response of an ionospheric plasma to incident EM waves. The code was used to investigate the mechanisms behind several recent experimental observations which have not been fully understood, including the effect of 2D density inhomogeneity on the O-mode to Z-mode conversion process and thus the shape of the conversion window, and the influence of EM wave polarisation and frequency on the growth of density irregularities.

Introduction

Investigating the fundamental mechanics of the ionosphere is an important and active area of Space Physics research. Ionospheric plasma physics is crucial to the communications industry: radio waves must cope with the ionosphere's reflective and refractive properties, satellite signals must pass through it; without a thorough understanding of the manner in which the ionosphere affects electromagnetic wave propagation, technology such as GPS would not be viable. Study of the ionosphere also presents the opportunity to investigate fundamental plasma physics over vast scale lengths and observe the diverse multitude of plasma waves and instabilities the ionosphere is capable of supporting. To this end, the ionosphere has been extensively studied though illumination via high-power, radio-frequency electromagnetic "pump" beams. Artificial ionospheric modification experiments of this type have observed of a wide range of complicated and often nonlinear plasma processes, many of which are highly sensitive to the polarisation, frequency or inclination angle of the incident electromagnetic waves, and all of which are greatly influenced by the background plasma density profile. The mechanisms behind many of these interactions are not fully understood, and would benefit from accurate numerical simulation of the underlying physical processes. Although substantial approximation and assumption is necessary in any simulation code, time-explicit computational experiments can offer a greatly enhanced time and spatial resolution when compared to real ionospheric measurements, allowing fine-detail investigation of wave and plasma behaviour. In a simulation, the initial conditions can be easily set and controlled; observation of a particular phenomenon is not reliant or contaminated by unpredictable background variability. Numerical calculations allow certain processes to be arbitrarily "switched on/off" by addition or removal of terms from the update equations, meaning that the dominant process responsible for a particular observed feature can be more easily disentangled form the many coupled processes involved in a wave-plasma interaction.
In this article we summarise the development and application of a GPU-accelerated finite-difference time-domain (FDTD) code designed to simulate the time-explicit response of an ionospheric plasma to incident electromagnetic (EM) waves, and the subsequent application of the new code to investigate the mechanisms behind several recent ionospheric-modification experimental observations which have not yet been fully understood or explained theoretically.

For a more detailed exploration of this work, please see thesis [4], or related publications [2], [3], and [9].

Computational Scheme

A key component of this research was the development of a new high-performance finite-difference time-domain code designed to simulate the response of a dynamic, magnetised and inhomogeneous ionospheric plasma to an incident radio-frequency electromagnetic wave. Although many excellent plasma codes already exist, none of the existing codes were explicitly tailored to the task of simulating an ionospheric heating experiment, incorporating the following crucial features in particular:

- The code was required to simulate not only the EM wave fields and multiple-fluid plasma velocities (as have been treated by previous FDTD schemes), but also the time-explicit perturbations to the plasma medium in response to an incident EM wave, thus allowing non-linear plasma processes to evolve naturally via the leap-frog time-stepping algorithm.

- Simulation runtimes must be kept realistically low, despite runs requiring the demanding combination of a sufficiently-large computational domain to model the ionospheric “interaction region” (domain dimensions of $> 1\,km$ scale) and sufficiently-fine resolution to accurately model radio-frequency EM and plasma waves (discrete grid steps of 10m scale or less).

- The code was required to simulate arbitrary, user-defined plasma density and temperature distributions with spatial variation in multiple dimensions, to allow the influence of structures such as density-depleted ducts and periodic density irregularities to be investigated.

The simulation scheme involved the finite-difference approximation of the coupled equations describing the propagation of EM waves and the time-dependent behaviour of a multiple-fluid plasma, following the well-established techniques described in, for example, [10], [11] or [12]. The effect on wave propagation due to the presence of plasma was introduced through the coupling of Maxwell’s wave equations with the Lorentz equations of motion, with fluid velocity component nodes spatially co-located with the electric field component nodes in the Yee cell and offset in time. Anisotropy was introduced through inclusion of a static externally-applied magnetic field. New time-advancement equations for the evolution of plasma fluid density and temperature (for both electrons and positively-charged ions) in the ionospheric F-region were included, allowing perturbations to the multiple-fluid plasma medium to be included in the time-explicit leapfrog update algorithm.
Accelerating the code using graphical processing unit (GPU) technology was demonstrated to significantly boost code performance: a dual-GPU implementation of the code was found to achieve a rate of node update almost two orders of magnitude faster than a serial CPU implementation. Optimisation techniques such as memory coalescence were shown to have a significant effect on the performance of the GPU code, and it was demonstrated that large performance gains could be achieved through careful choice of the GPU work group dimensions.
Numerical validation tests were performed in which FDTD scheme was shown to achieve a good agreement with both the predictions of plasma theory and the results computed using a commercially-available software package, which was used as a benchmark. Of particular relevance, the propagation characteristics of ordinary-mode (O-mode) and extraordinary-mode (X-mode) EM waves in an inhomogeneous, magnetised plasma were accurately replicated, including the formation of a high-amplitude Airy-like standing wave below the O-mode reflection height.
Once validated, this code was used to investigate several unexplained plasma processes observed during recent ionospheric modification experiments, as described below. Although this code was designed to be suitable for the simulation of wave-plasma interactions in the F-region of the ionosphere, it could also with minimal modification be applied to investigate many other situations for which a fluid description of the plasma is appropriate , such as to study fluid-type wave behaviour in the magnetosphere or solar wind.

The work describe in this section has been published as part of [2].

Simulation of the Radio Window and Magnetic Zenith Effect

The magnitude of the plasma perturbation induced during artificial ionospheric modification experiments has been observed to depend strongly on the inclination angle of the electromagnetic pump beam. [5] proposed that this Magnetic Zenith Effect is due to the O-mode to Z-mode conversion process that can occur in the F-region for a narrow range of pump wave inclination angles, which allows an incident O-mode-polarised wave to propagate beyond the expected O-mode reflection layer as a Z-mode wave. However, the greatest plasma perturbations have often been observed to occur not for pump waves inclined at the Spitze angle (at which conversion to the Z-mode is theoretically most favourable), but for wave angles somewhere between the Spitze and the magnetic field directions (see, for example, [6]). This suggests that the conversion process, and the "Z-mode window" for which conversion is likely to occur, may be modified by the presence of 2D inhomogeneities in the ionospheric plasma density close to the interaction region.

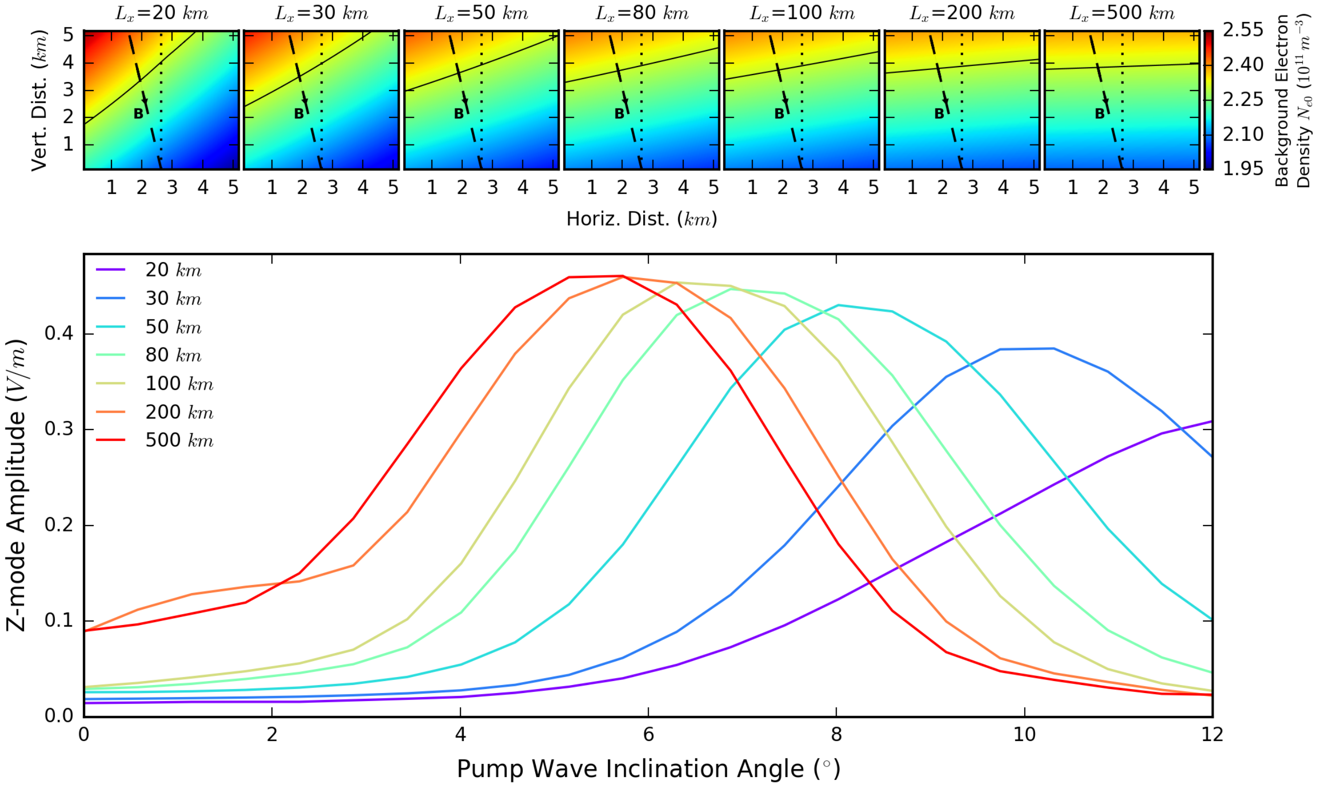

Figure 1: Simulated Z-mode window for varying background horizontal plasma density slope scale size L_x (smaller L_x implies a steeper slope). Each curve shows the amplitude of EM waves propagating beyond the O-mode reflection height as a Z-mode wave, for a range of initial O-mode beam angles. It can be seen that increasing the steepness of the slope shifts the centre of the radio window away from the Spitze direction ($\sim 5.5°$) and towards the magnetic zenith direction ($\sim 12°$). The background plasma density, magnetic field direction (dashed line), vertical direction (dotted line) and position of the O-mode reflection height (solid black line) used for each L_x are shown in upper panels. *Figure originally published in [3].*

The FDTD code was used to investigate influence of 2D density variations on the O-mode to Z-mode conversion process, and the contribution of this process to several aspects of the observed Magnetic Zenith Effect. This conversion process has previously been investigated theoretically for the case of a 1D variation in electron density; the new code allowed this process to be investigated numerically for the case of a 2D plasma density profile for the first time.

The simulations demonstrated that the angular window for O-to-Z-mode conversion is highly sensitive to the form of the 2D electron density profile. In particular, addition of a linear horizontal gradient was found to shift the centre of the conversion window away from the Spitze direction and towards the geomagnetic field-aligned direction, with a steeper slope found to produce a greater shift in position, as shown in Figure 5. A shift of this kind could explain why the most significant plasma modification has been experimentally observed for pump wave directions between the Spitze and field-aligned angles.

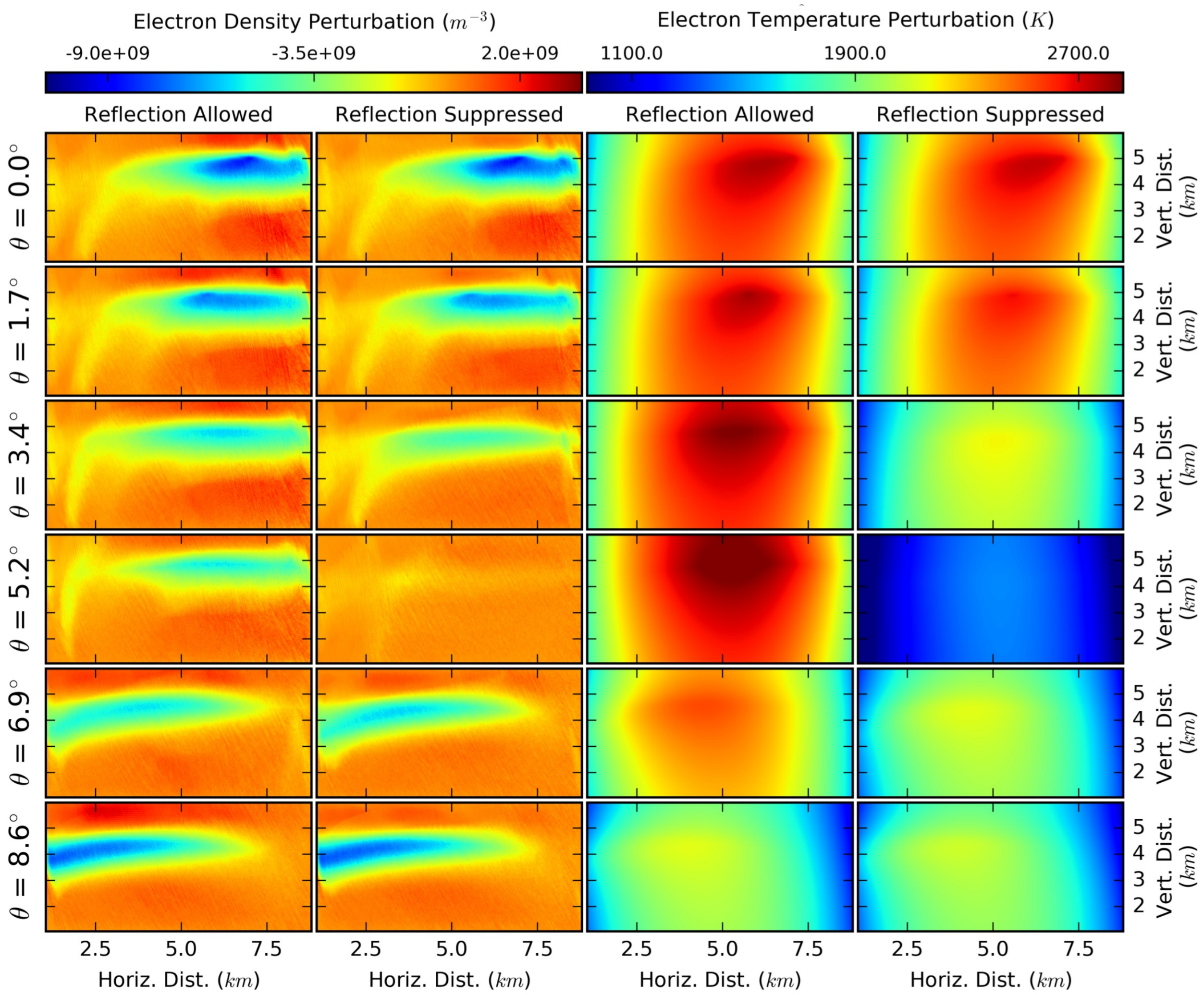

Figure 2: Variation of simulated electron density and electron temperature perturbation with pump wave inclination angle, for the cases that Z-mode reflection is allowed and Z-mode reflection is suppressed. In the reflection-allowed scenario, the strongest electron temperature enhancement was found to occur for the pump wave inclined an angle of $5.2°$ (close to the Spitze angle), supporting the argument that the pump wave that is most effectively converted the Z-mode excites the greatest temperature perturbation. The lowermost panels show the variation of the maximum value of electron temperature enhancement and electron density depletion in the simulation domain with time, for the Z-mode reflection allowed (solid lines) and suppressed (dashed lines) scenarios. Background conditions are shown in the uppermost panel. *Figure originally published in [3].*

The contribution of the O-mode to Z-mode conversion process to the large-scale modification of ionospheric plasma was investigated by comparing simulations in which the Z-mode wave was allowed to reflect back towards the interaction region to simulations in which the Z-mode was absorbed before reflection by an artificial perfectly-matched layer. Allowing the Z-mode wave to reflect was found to cause enhancement of the electric field in a resonant layer normally inaccessible to extraordinary-mode waves, leading to a substantial increase in electron temperature enhancement around the interaction region. For the case of a vertical electron density profile and a Spitze-directed wave, electron temperature enhancement was found to be more than a factor of 2 greater with Z-mode reflection allowed than when it was suppressed. The O-mode to Z-mode conversion process was shown to result in an angular dependence in electron temperature enhancement, as the angles for which conversion of the pump wave to the Z-mode were more favourable were found to correspond to greater temperature gains, as shown in Figure 6. The inclusion of 2D inhomogeneities was also found to influence the variation of electron plasma perturbation with pump wave angle, corresponding to the associated modification of the radio window.

The simulation results demonstrated that the presence of 2D density inhomogeneities around the O-mode reflection height can significantly modify the angular shape of the Z-mode conversion window, and that the excitement and subsequent reflection of Z-mode waves can lead to substantial enhancements in artificially-induced plasma perturbations. In combination, these processes cause the magnitude of thermal plasma perturbation to depend strongly on both the pump wave inclination angle and the 2D electron density profile. This offers a potential mechanism behind several features of the observed Magnetic Zenith Effect.

The work describe in this section has been published as part of [3].

Simulation of Density Irregularity Growth During O-Mode and X-Mode Heating

Anomalous processes involving the excitation of electrostatic (ES) plasma waves are a key component of F-region ionospheric modification when using O-mode waves. These processes have been shown to be particularly sensitive to the proximity of the pump wave frequency to harmonics of the electron gyrofrequency (see, for example, [8]). Recent ionospheric heating experiments performed at the EISCAT heating facility in Troms using X-mode waves have also observed several anomalous plasma effects previously associated with O-mode waves only, including large-scale temperature enhancement and generation of field-aligned density irregularities (see, for example, [1]).

Inclusion of time-explicit electron and ion density perturbations in the FDTD time-stepping algorithm allowed the growth of the small-scale geomagnetic field-aligned density irregularities associated with anomalous plasma heating to be investigated numerically. The FDTD code was employed to simulate ionospheric modification experiments using both O-mode and X-mode polarised pump waves of varying frequencies, and demonstrated that both polarisations are capable of exciting several bands of field-aligned density-depleted irregularities, predominantly located at points where the background electron plasma frequency was closely matched with a harmonic of the electron cyclotron frequency, as shown in Figure 3. Comparing simulations in which ion motion was allowed or suppressed indicated that a parametric process was responsible for the production of these irregularities, possibly involving the excitement of perpendicularly-propagating ES waves such as Bernstein modes.

The numerical code was modified to take into account an estimation of the ES fields associated with any excited density irregularities. Inclusion of these fields as a source term in the temperature update equation was shown to result in a greater increase in the simulated electron temperature than was produced in simulations performed where only the FDTD electromagnetic E-fields were considered. These temperature enhancements were found to be in reasonably good agreement with the anomalous heating predicted using the equations of [7].

Plasma-wave driven anomalous heating processes associated with the growth of irregularities of this nature could potentially explain the observations of both significant temperature enhancements and the growth of field-aligned density irregularities during X-mode experiments at EISCAT. The growth of irregularities close to the third gyroharmonic height could also explain an observed asymmetry in anomalous absorption observed during O-mode experiments.

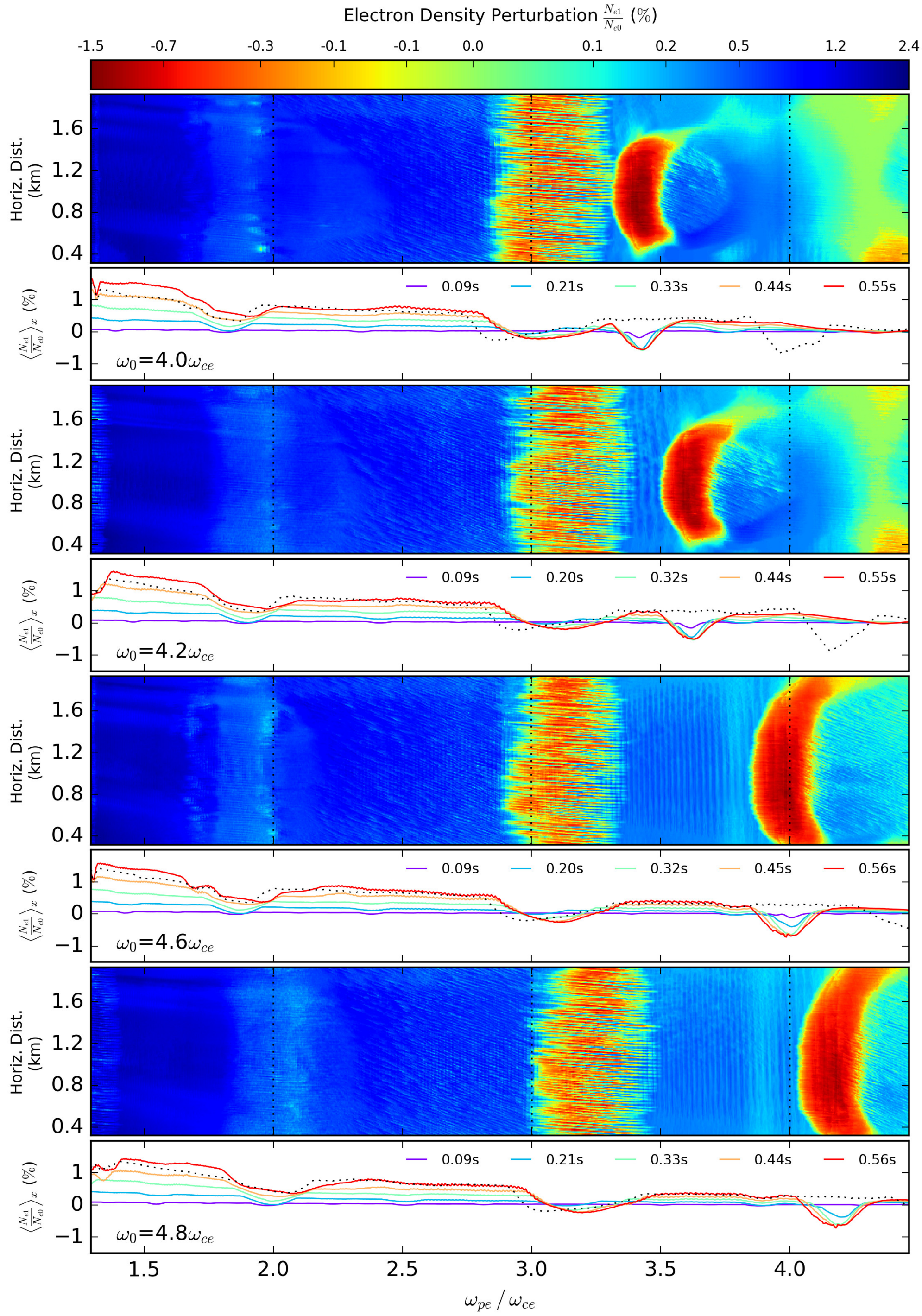

Figure 3: Examples of the density perturbations developed in the FDTD simulation using X-mode pump wave frequencies in the range $(4-5)\omega_{ce}$, where ω_{ce} is the electron gyrofrequency. For each pump frequency, the upper panel displays the spatial snapshot of the electron density perturbation developed after $0.56, s$. Note that the colour-map has been logarithmically-normalised. The gyroharmonic heights, at which the background electron plasma frequency corresponds to an electron gyroharmonic frequency, are indicated by dotted lines. A large density depletion can be seen at the X-mode wave reflection layer. Populations of electron density striations, elongated along the imposed geomagnetic field direction, can be seen to grow close to these gyroharmonic height (particularly just above the third gyroharmonic height in this case). The lower panel for each frequency shows horizontally-averaged vertical profiles of the density perturbation for a range of heights (solid lines). The horizontally-averaged profile from the corresponding O-mode simulation is indicated by the dotted line (recorded after $0.56, s$ simulated time).

Comparison of Simulated X-mode Wave Fields with Theoretical Parametric Instability Thresholds

The thresholds for excitation of several parametric instabilities were analysed for the case of an X-mode polarised pump wave by [9]. The calculations demonstrated that it is possible for these processes to be excited during X-mode heating, provided a minimum fraction of the pump wave power was directed along the geomagnetic field direction. A perfect X-mode wave would have no component of its wave field directed along this direction. However, the ionosphere is an inhomogeneous, dispersive and anisotropic medium, and it is possible that a non-zero parallel component of the pump field can arise due to the dispersion or refraction of the wave by the ionospheric plasma.
The FDTD code was used to simulate the modification of the pump wave field by the ionospheric plasma for the conditions experienced during several X-mode heating experiments. The simulation results demonstrated that in certain cases the theoretical E-field threshold required for the excitation of the parametric instabilities was exceeded in a region below the X-mode reflection height, as shown in Figure 4, in good agreement with the experimental observations of HF-enhanced plasma and ion lines. Excitation of such instabilities and the resultant anomalous plasma heating could contribute to the large scale plasma modification recorded during X-mode heating experiments at the EISCAT heating facility. Parametric decay of the pump wave to plasma waves could also help explain the excitation of density irregularities by X-mode waves seen in the previous simulation study described above.

The work described in this section has been published as part of [9].

Conclusions

Ionospheric modification by means of high-power electromagnetic (EM) waves can result in the excitation of a diverse range of plasma waves and instabilities. In this article we summarised of the development and application of a GPU-accelerated finite-difference time-domain (FDTD) code designed to simulate the time-explicit response of an ionospheric plasma to incident EM waves. The code was used to investigate the mechanisms behind several recent experimental observations which have not been fully understood, including the effect of 2D density inhomogeneity on the O-mode to Z-mode conversion process and thus the shape of the conversion window, and the influence of EM wave polarisation and frequency on the growth of density irregularities. The O-to-Z-mode conversion process was shown to be responsible for a strong dependence of artificially-induced plasma perturbation on both the EM wave inclination angle and the 2D characteristics of the background plasma. Allowing excited Z-mode waves to reflect back towards the interaction region was found to cause enhancement of the electric field and a substantial increase in electron temperature. Simulations of O-mode and X-mode polarised waves demonstrated that both are capable of exciting geomagnetic field-aligned density irregularities, particularly at altitudes where the background plasma frequency corresponds to an electron gyroharmonic. Inclusion of estimated electrostatic fields associated with irregularities in the simulation algorithm resulted in an enhanced electron temperature. Excitation of these density features could address an observed asymmetry in anomalous absorption and recent unexplained X-mode heating results reported at EISCAT. Comparing simulations with ion motion allowed or suppressed indicated that a parametric instability was responsible for irregularity production. Simulation of EM wave fields confirmed that X-mode waves are capable of exceeding the threshold for parametric instability excitation under certain conditions.

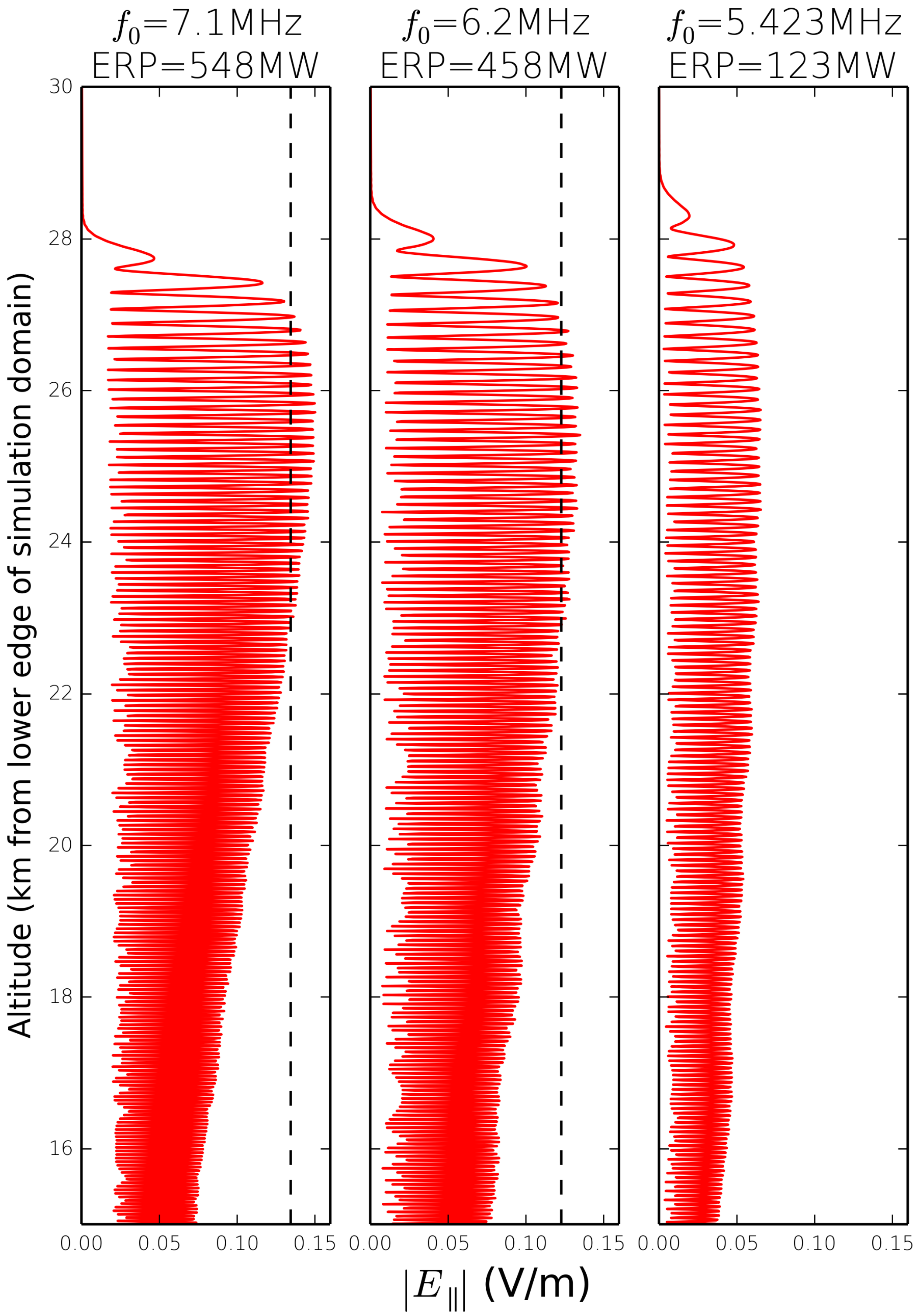

Figure 4: The simulated $E_{\parallel}$ amplitude around the X-mode reflection height for several sets of experimental conditions, averaged over 2×10^5 timesteps ($\sim 2.67\,ms$). The field amplitude required for parametric instability excitation as calculated by [9] is indicated by a dashed line. For the experimental conditions shown in the leftmost and centre panels, the simulation results indicate that the parametric instability threshold could be exceeded in a region just below the X-mode reflection layer ($\sim 28\,km$ from the lower edge of the simulation). For the conditions shown in the rightmost panel, the instability threshold corresponded to $\sim 50\%$ of EPR and therefore was much higher than the maximum simulated E-field amplitude shown here. *Figure originally published in [9].*

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Computational Physics Group News

- ## The Computational Physics Annual PhD Thesis Prize

Each year, the IoP Computational Physics Group awards a Thesis Prize to the author of the PhD thesis that, in the opinion of the Committee, contributes most strongly to the advancement of computational physics.

The winner of this year's Thesis Prize is Ioan Magdau for his thesis entitled "Theoretical Investigation of Solid Hydrogen and Deuterium", which was undertaken at the University of Edinburgh.

Runner-up prizes are awarded to Ahmed Al-Refaei, for his thesis entitled "Efficient Production of Hot Molecular Line List", carried out at UCL, and Morgane Vacher, for her thesis entitled "Electron and Nuclear Dynamics Following Molecular Ionization: Computational Methods and Applications", carried out at Imperial College London.

Thanks to the generosity of AWE (`http:www.awe.co.uk`) Ioan receives £300 and Ahmed and Morgane receive £100 each for their achievements. Details of their work will be reported in forthcoming issues of the group newsletter.

The deadline for the 2018 prize is 30th April 2018 and details are available at the following link:
`http://www.iop.org/activity/groups/subject/comp/prize/page_40691.html`

Applications are encouraged across the entire spectrum of computational physics. Entry is open to all students from an institution in the UK or Ireland, whose PhD examination has taken place since 1st January 2017 and up to the submission deadline, and who did not apply for the CPG Thesis Prize in the previous year. Prize winners will be invited to write a feature article in the Computational Physics Group newsletter.

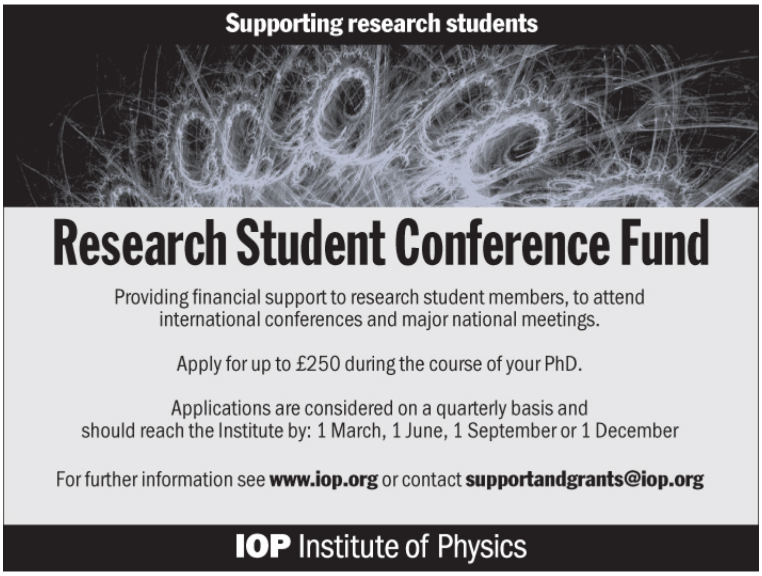
Candidates are asked to note that if a similar thesis prize is offered by another IOP group (such as the Theory of Condensed Matter group), the Committee intends to liaise with that group so that both prizes will not be awarded to the same applicant.

The submission format is as follows:

- A four page (A4) abstract describing the background and main achievements of the work
- A one page (A4) citation from the PhD supervisor
- A one page (A4) confidential report from the external thesis examiner

Entries (PDF documents preferred) should be submitted by email, with "IOP CPG Thesis Prize" as the subject header, to Dr Arash Mostofi (a.mostofi@imperial.ac.uk). Any queries should also be directed to Dr Arash Mostofi. A few more details, including a list of past winners, can be found on the group webpage `http://www.iop.org/activity/groups/subject/comp/prize/page_40691.html`.

- **IoP Computational Physics Group - Research Student Conference Fund**



The Institute of Physics Computational Physics Group is pleased to invite requests for partial financial support towards the cost of attending scientific meetings relevant to the Group's scope of activity. The aim of the scheme is to help stimulate the career development of young scientists working in computational physics to become future leaders in the field.

Further details on this award can be found at:

`www.iop.org/about/grants/research_student/page_38808.html`

Conference and Workshop reports

- **Quantum Plasmonics (QUPLA) workshop 2016**

24-26 August 2016 at Imperial College London.

Plasmonics is a recent discipline focused on the study of the interaction of light with matter, such as metal nanoparticles or metallic surfaces, where surface plasmons polaritons (SPPs) play a fundamental role. SPPs are mixed states between collective electron density excitations and light that are confined to the interface between a metal and an insulator. These excitations are extremely important because of their potential for nanotechnological applications. In fact, SPPs have a nanometric spatial confinement that is crucial for the development of devices smaller than 100 nm. For example, an important goal of plasmonics is to replace electronics technology with plasmonics offering faster responses resulting from the light properties of SPPs.

In the last few years, mainly because of advances in nanofabrication, interest in plasmonics moved towards the properties of very small nanoparticles systems. In such systems, a new challenge arises, the appearance of quantum effects. In fact, until now, plasmonics has been mainly based on classical physics concepts.

The main goal of QUPLA was to initiate a discussion and an exchange of ideas between researchers who model plasmonic systems, but from different points of view, namely plasmonics and electronic structure theory.

The most pointed topic was the difference between the various plasmon families (localized, propagating or bulk plasmons) and how to simulate them, a concept a bit unclear in the electronic structure community. Several discussions followed on how to attack the quantum computation problem of many electrons when the size is too big for a usual first-principles density-functional theory (DFT) approach. Probably the most acclaimed suggestion was one that attempts to divide the problem in two parts: the internal part of a metal nanoparticle can be calculated considering a bulk system, for which easy solutions are possible, while the surface has to be properly done with DFT or post-DFT methods (such as the GW approach).

It is important to point out that recently there have been significant efforts to include quantum effects in classical plasmonics. Such approaches either modify the classical Maxwell equations of electrodynamics by introducing, for example, nonlocal, nonlinear and quantized fields, or "borrow" quantization techniques used in empty cavities in quantum optics. However, such ad hoc approaches are fundamentally unsatisfactory and novel, microscopically accurate descriptions of plasmonic systems that include quantum effects is sorely needed.

On the other hand, the scope of first-principles theoretical approaches that aim at a parameter-free quantum-mechanical description of materials has increased drastically in recent years. Algorithmic and technological advances allow for the modelling of relatively large systems comprising thousands of atoms using density-functional theory. Moreover, several techniques for the description of electronic excitations are available, such as time-dependent DFT and many-body perturbation theory (GW/Bethe-Salpeter approach). With these advances, we expect that first-principles approaches can contribute to the understanding of plasmonic systems and become valuable additions to the toolkit of researchers in the field.

It is important to point out, however, that while such first principle approaches describe the properties of electrons with high accuracy, the description of light is typically simplified. Moreover, the modelling of large clusters containing millions of atoms is currently still out of reach for these methods.

This above discussion clearly highlights the need for the development of new approaches for the theoretical description of plasmonic systems. We have identified a strategic and significant opportunity to overcome this challenge by converging classical electrodynamics approaches, quantum-mechanical electronic structure theory and quantum optics methods from opposite length scales at the nanometer regime.

In summary, different disciplines are studying physical phenomena in plasmonic systems, but from different, often complementary points of view. The description of light-matter interactions in small nanoparticles, where quantum effect becomes important, poses a significant challenge to all approaches. This workshop initiated an exchange of ideas to identify routes towards a complete and microscopically accurate description of plasmonic phenomena. In fact, we strongly believe that all what we need is to make the plasmonic and electronic structure to interact!

Acknowledgements The organizers are grateful to the Psi-k Network (`http://www.psi-k.net`), the JCMaxwell node of CECAM (`http://www.cecam.org`), Imperial College London and the Computational Physics Group of the Institute of Physics for funding.

Report kindly provided by Dr Vincenzo Giannini, Imperial College London.

- **Euro-TMCS II:Theory, Modelling and Computational Methods for Semiconductors**

  7-9 December 2016 Tyndall National Institute, University College Cork.
  Website: `http://www.tmcsuk.org/conferences/Euro-TMCSII/` .

Figure 5: Euro-TMCS II, during lecture.

Organized by Dr. Prof Stanko Tomic, Prof. Eoin O' Reilly and Dr Stefan Schulz, the meeting has provided a platform for presentation of the current state-of-the-art computational methods in semiconductor physics like, with 5 invited presentations, 15 oral and 15 poster presentations (see Figure 5). divided into six sessions titled 2-D materials, Nanostructures & Poster Pitches, DFT & Fundamentals, New Materials, Hybrid Perovskites & Solar Cells and Device Simulations. Particular success of the meeting was the training day (day 1), attended by over 40 researchers from Ireland, the UK and the rest of Europe. Subjects covered by tutorials were: Plane-Wave DFT and LDA, DFT-Tight-Binding Theory, Modelling of Halide Perovskites, Multiscale Device Simulations and Non-equilibrium GreenâĂŹs Function Methods. The commercial company TiberLab was present at the meeting, giving an overview of multiscale device simulation on the training day and also presenting some of their simulation results during the meeting. This inclusion of industry participants has always been a valued part of the TMCS conference series, ensuring that the meeting covers the full spectrum from forefront ab-initio calculations through to commercial application. We have also published the conference abstracts booklet (available on request). In addition, details of the conference remain available at http://www.tmcsuk.org/conferences/Euro-TMCSII/ . Organisation/hospitality wise we believe the meeting went smoothly. The tutorial day was hosted in Tyndall National Institute, while the 1.5 days of presentations took place in the Aula Maxima in University College Cork. The conference dinner took place in the city centre (Imperial Hotel), so that attendees could also spend time to experience the wider aspects of the city (Figure 6).

Figure 6: Euro-TMCS II reception.

Report kindly provided by Dr. Prof Stanko Tomic for Euro-TMCS II.

- ## TYC-Toucan workshop on shaping Nanocatalysts

14-16 Decembre 2016 at King's College London.
Website: `http:www.thomasyoungcentre.org/events/energy-materials-workshop`

Chaired by Dr. Francesca Baletto, hosted the 4_{th} TYC Energy Materials Workshop jointly to the Toucan International conference from 14-16 December 2016. The workshop brought together the leading experts from across the world on the design of nanocatalysts and plasmonic nanoparticles for catalytic applications. Prof. Peter Main, Head of Physics Department and IoP fellow, opened the conference, while prof. Gianfranco Pacchioni (Univ. of Milan) gave the closing remarks.

79 participants from institutions spread over 14 different countries attended the conference and at least a 20% were female scientists. In the previous editions, the workshop was attended by a similar number of participants. The main sponsors were Psi-K, CCP9 and EPSRC throughout the critical mass network, Toucan. A special issue of the EPJB will also result from the conference later this year. A bets poster prize, offered by Springer, was awarded to Mr. Jolyon Aarons (Univ. of Southampton). The IoP contribution made possible to lower significantly the registration fees for students. This makes the workshop easily accessible and 43% of the audience was made by PhD students. During the first day students were gently introduced to the main topics thanks to longer and educational talks provided by the Toucan team. They have also the chance to meet the CEO of Overleaf who gave a talk on the transition from academia to industry.

The workshop not only brought together experimentalists and modellers, but thanks to the warm and nice atmosphere delegates shared their scientific views, and techniques and boost their collaborations. As Pacchioni highlighted in his closing remarks,“we have learnt something new in those days, and this is not so common”.

Unfortunately, due to a technical problem, no photos were taken during the workshop.

Report kindly provided by Dr. Francesca Balletto, Chair of TYC-Toucan workshop on Shaping Nanocatalysts.

- **Conference on Computational Optical Sensing and Imaging, part of Imaging and Applied optics congress 2016**

25-28 July 2016 at Kongresshaus Stadthalle Heidelberg, Heidelberg, Germany

Highlights. The keynote lectures were of high quality and focused on various areas of optics. Especially Prof. Chris Dainty spoke about his 50 years of experience working in optics which was interesting and motivating at the same time. There was an interesting discussion session about how computer vision scientists and computational optics scientists can work together to increase the productivity and bring them closer. This session was led by Dr. Ram Narayanswamy from Intel. There was a careers in optics session organized as a part of OSA 100 years celebration events. The panel consisted of all the three keynote speakers who spoke about their careers and how they had to make decisions which were key in their careers. All three coming from different backgrounds made the session more informative. They have also gave some general advice for early career researchers which I found very useful in my case particularly since I am approaching towards the end of my PhD. Benefits: There were numerous invited and contributed talks which were in my research area of Fourier Ptychography. This helped me to broaden my knowledge in the area and get to know the current research being carried out by other researchers in the field. My talk was attended in large number and received a lot of interest. I had a chance to talk to two other research groups who contributed largely in my research area. They both appreciated my talk and we had a discussion about potential future collaborations. It was a good opportunity for me to network with the forefront researchers in my area. Overall I think that the conference was a huge success. It was attended in large numbers and consisted plenty of interesting and useful invited and contributed talks. There were two additional invited talks presented by Prof. Joseph Izatt and Dr. Bernard Kress about future of optics in next 100 years organized part of OSA's 100 year celebrations. I felt they might be of interest to general audience along with Prof. Chris Dainty's key note talk.

Report kindly provided by Pavan Chandra Konda, PhD student, School of Physics and Astronomy at University of Glasgow

- **8^{th} Multiscale Materials Modeling international conference, 2016.**

8-14 October 2016 at Dijon, France.

Highlights. Attending the 8th international Multiscale Material Modelling conference was a fruitful experience for my personal and professional development. The principal motivation which brought me to join this conference was the symposium on the “Multiscale modeling of nanoalloys and metal-based nanohybrids” where I had the chance to listen to the work presented by leading scientist in the field of cluster science and further had the honour of presenting my own research outcomes. Of particular interest was the invited lecture by Prof. Richard Palmer from Birmingham University, where he addressed the need to consider shape fluctuations as phenomena which are often disregards in the field due to their complexity and yet significantly affect nanoclusters application in nanocatalysis and biomedicine. He further described in great detail how cutting-edge techniques actually enable dynamical manipulation of size-selected clusters so to have control on their chemophysical properties. His fascinating talk was then shortly after followed by my own presentation regarding the use of insilico approaches to predict structural metastability of metallic nanoclusters: by means of numerical approaches we unveiled and rationalized the complex dependence of the accessible rearrangement pathways of magic-size transition metals nanoclusters on their size, composition and interatomic potential interaction. My work gauged interest both from an experimental and theoretical perspective. The transferability of the applied techniques to larger size systems and more complex processes has been questioned and fertile discussions and possible collaborations raised. Being able to further attend other presentations from scientist outside my area of specialization broaden my horizons and, in particular, enabled me to develop my knowledge in data driven analysis and material screening for the rational design of new materials. Prof. Claudia Draxl plenary talk on discussed on such approaches and their use targeted to characterize the relevant properties of many different materials in a systematic manner so to obtain insights by means of statistical learning methods which would otherwise be unseen by human pattern recognition. Overall, attending MMM conference has been a pleasure because of the fascinating science presented and its great location, Dijon being a UNESCO heritage site. Thus I am grateful to IOP computational physics group for his generous support.

Report kindly provided by Kevin Rossi, PhD student,King's College London, Physics Department, Strand, London, UK

• Computing in Cardiology 2016

11-14 September 2016 at Simon Fraser University, Vancouver, Canada.

Highlights. I would like to begin this report by thanking the Computational Physics Group for their sponsorship, which was instrumental in allowing me to attend the Computing in Cardiology conference this year in Vancouver, Canada. It was a busy conference with approximately 400 attendees. A large variety of topics were covered in both oral and poster sessions, such as membrane and cellular models, imaging techniques and analytical software to name but a few. One presentation even involved the use of virtual reality headsets to explore a virtual, 3D, contracting heart. There were also several social events intended to foster collaboration, including a bike ride around Stanley Park, a formal dinner and a hike up Grouse Mountain. Guest speakers during the Sunday Symposium included Robert Thirsk, Peter Norsk and Pierre-Francios Migeotte amongst others. My talk, which was entitled 'Modelling the Effects of Nifedipine on Ventricular and Myometrial Cells of Pregnant Rats', was well received. I was particularly pleased with the questions asked by audience members, who included some prolific contributors to the field, such as Blanca Rodriguez (Professor of Computational Medicine, Oxford) and Eleonora Grandi (Assistant Professor of Pharmacology, UC Davis). Blanca made an important point about the significance of sodium channel block to contraction in the heart, which I intend to investigate with my models. Another interesting point was made by Gary Mirams (College Lecturer, Oxford) regarding the kinetics of nifedipine and how they may partly explain the differences in action between the heart and uterus. During the conference I also had the honour of chairing a session in the stead of my supervisor, as he was unable to attend. The session was dedicated to ECG imaging, a topic I have a growing interest in due to my efforts to simulate similar techniques related to processing uterine electrical activity. I had to introduce the session and speakers, as well as manage questions from the audience and ask my own in their absence. There were many sessions related to my work, but one of particular interest was focused on foetal, antenatal and neonatal cardiovascular control. It was fascinating to learn about contemporary techniques in reading the heart activity of unborn children and how such information can be of use to clinicians. Overall I'd describe the conference as a great success, both for advancing the field and for myself, personally. Vancouver is a beautiful setting for a conference and I'd highly recommend a visit to the city. I am very grateful for the opportunity to have attended CinC 2016 and look forward to implementing the results of discussions I had while I was there.

Report kindly provided by Craig Testrow, PhD student, at The University of Manchester

Upcoming Events of Interest

Upcoming events of interest to our readers can now be found via the following web links.

- IOP's index page for scientific meetings, including conferences, group events and international workshops:

  `www.iop.org/events/scientific/index.html`

- IOP Conferences page for conference information, calendar and noticeboard:

  `www.iop.org/events/scientific/conferences/index.html`

- All events being run or supported by IOP Groups including calendar and links to event web pages:

  `www.iop.org/events/scientific/group/index.html`

- Thomas Young Centre: The London Centre for Theory and Simulation of Materials organises many different kinds of scientific events on the theory and simulation of materials, including Highlight Seminars, Soirees and Workshops. For further details of upcoming events please visit:

  `www.thomasyoungcentre.org/events/`

- CECAM is a European organization devoted to the promotion of fundamental research on advanced computational methods for atomistic and molecular simulation and their application to important problems in science and technology. CECAM organises a series of scientific workshops, tutorials and meetings. For further details please visit:

  `www.cecam.org`

Computational Physics Group Committee

The current members of the IoP Computational Physics Group committee with their contact details are as follows:

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Some useful web links related to the Computational Physics Group are:

- CPG webpages
  `comp.iop.org`
- CPG Newsletters
  Current issue:
  `www.iop.org/activity/groups/subject/comp/news/page_40572.html`
  Previous issues:
  `www.iop.org/activity/groups/subject/comp/news/archive/page_53142.html`
  `www.soton.ac.uk/~fangohr/iop_cpg.html`

Related Newsletters and Useful Websites

The Computational Physics Group works together with other UK and overseas computational physics groups. We list their newsletter locations and other useful websites here:

- Newsletter of the Computational Physics Division of the American Physical Society:
  `www.aps.org/units/dcomp/newsletters/index.cfm`
- Europhysicsnews newsletter of the European Physical Society (EPS):
  `www.europhysicsnews.org/`
- Newsletter of the Psi-k (Ψ_k) network:
  `www.psi-k.org/newsletters.shtml`