IOP Institute of Physics
Computational Physics Group

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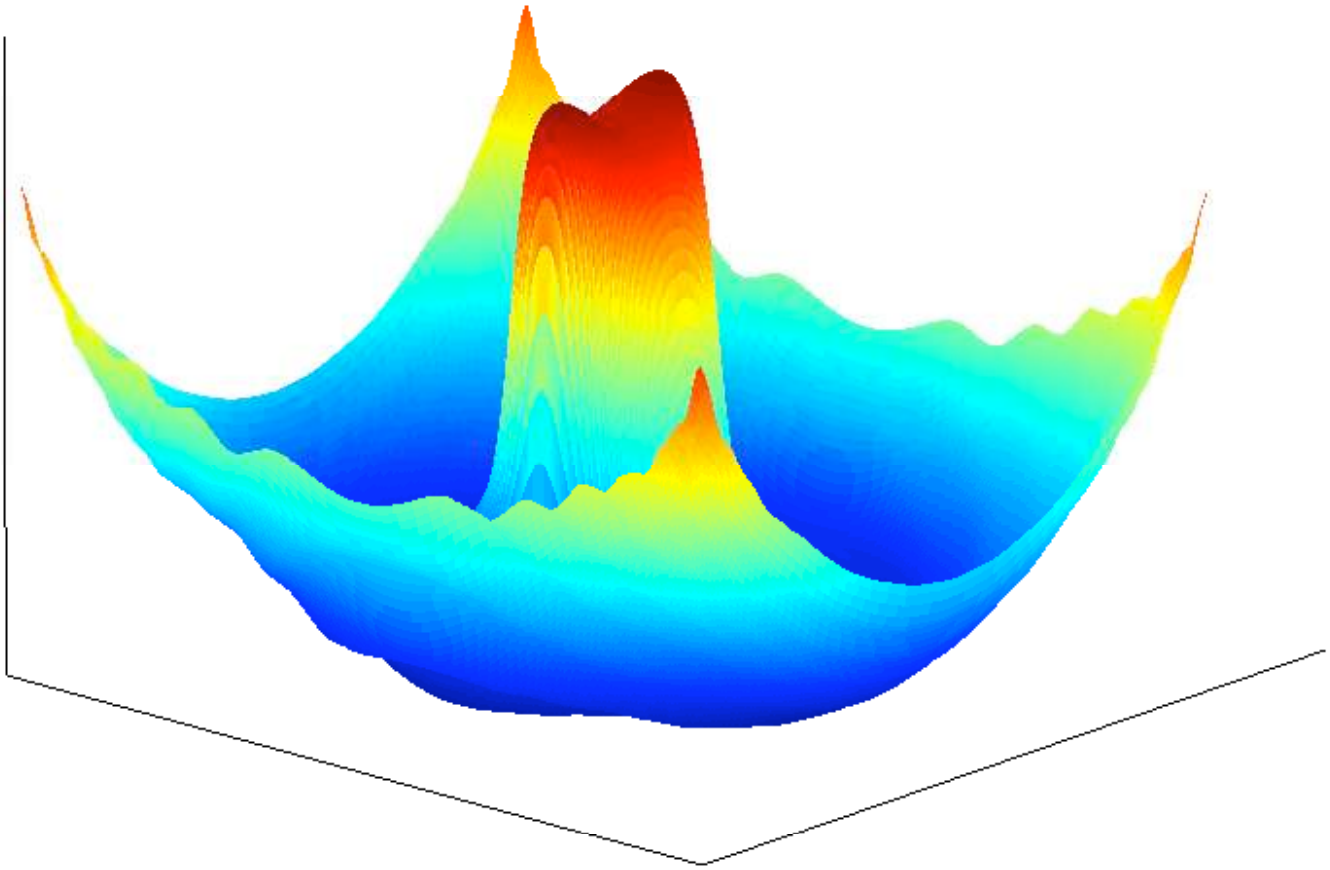
Newsletter



Modelling of Liquid Crystal Devices

Newsletter Contents

Figure on cover:
Phase of a Gaussian beam inside a liquid crystal cell is undergoing changes that ultimately lead to an optical singularity at the exit from the cell. See article beginning on page 1.

This Newsletter . . .

Dear Newsletter Readership,

this is the second newsletter that is distributed exclusively electronically. This and older versions of the newsletter are available electronically. We note that all http links in the newsletter are clickable. This has been so for many years, but becomes now more valueable as, presumably, more people will read the newsletter online.

The *main feature* (page 1) of this newsletter is provided by Dr Vera Hazelwood, the winner of the Computational Physics Group Thesis prize 2007.

As always, we value your feedback and contributions (email to Hans Fangohr at `fangohr@soton.ac.uk`).

The Computational Physics Group Committee.

Vortex optical singularities induced by a liquid crystal

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This short paper summarises one of previously unpublished chapters of my thesis titled "FDTD modelling of light interaction with liquid crystal devices" awarded in 2006.

Introduction

Liquid crystals are fascinating optical media. Physically they consist of spatially anisotropic molecules. The most common shapes are rods or discs. One of the simplest types of liquid crystals are nematics, which molecules are rod-like and arranged in a way that they have the orientational order, *i.e* all molecules are aligned along a particular direction, called the *director*. Nematics therefore posses spatial anisotropy, which leads to anisotropy of physical properties, and in particular, optical properties.

The nematic behaves as anisotropic crystal, exhibiting different refractive indices for different polarisations of light. Light polarised perpendicular to the optical axis feels the ordinary refractive index n_0, while light polarised parallel to the optical axis feels the extraordinary refractive index n_e.

Materials that have two refractive indices are said to be birefringent. Birefringence plays an extremely important role in all liquid crystal devices.

In order to construct a liquid crystal device, liquid crystal material must be put in cells. The chemical interaction of liquid crystal molecules with the cell substrates surfaces determines their orientation at the surface. Several possible cases are illustrated in Fig. 1. Fig. 1a shows the case when molecules are aligned parallel to the surface. Fig. 1b shows the case when molecules are aligned perpendicular to the surface. Fig. 1c shows the case when molecules are aligned at some arbitrary angle ϕ to the surface. Introducing another cell substrate, also introduce interaction with it and the overall arrangement of the molecules is determined from the minimum of the elastic free energy of the system. Fig. 2 illustrates two possible cells. In Fig. 2a both substrates make molecules to align perpendicularly. This results in the uniform molecule orientation. In. Fig. 2b the lower substrate orients molecules perpendicularly, while the upper substrate orients molecules parallel. This results in a twisted molecular orientation.

Usually, an external electric or magnetic field is also applied to the cell. Under certain conditions this application results in the reorientation of the liquid crystals molecules. The final orientation is again determined by the minimum of the free-energy, which apart from elastic part now includes the field interaction part. A wide variety of electric and magnetic phenomena has been experimentally observed and theoretically studied in liquid crystals in [1].

Liquid crystals also respond to light, as light is the electromagnetic wave. However, the interaction with light is more complex than the interaction with constant electric of magnetic fields. This is due to liquid crystals being birefringent, *i.e* affecting prop-

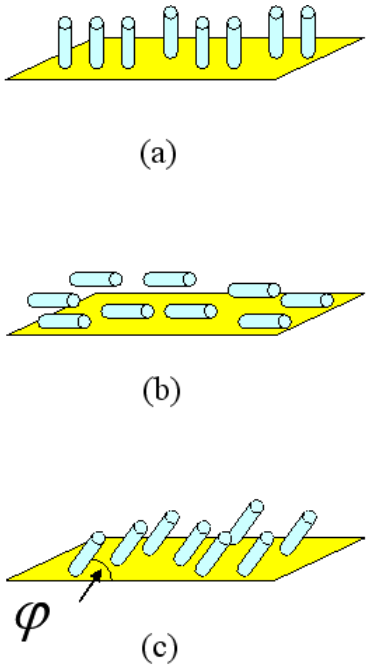


Figure 1: Different possible orientations of liquid crystals molecules at the cell surface. (a) - all molecules are perpendicular to the surface, (b) - all molecules are parallel to the surface, (c) - molecules are aligned at an arbitrary angle ϕ to the surface.

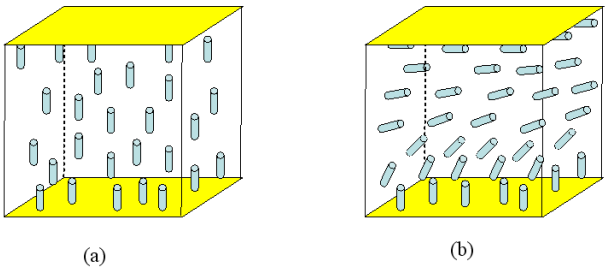


Figure 2: Liquid crystal in cells, (a) - both substrates align molecules perpendicular to their surface resulting in the uniform molecular orientation, (b) - the lower substrate orients molecules perpendicularly, while the upper substrate orients molecules parallel resulting in a twisted molecular orientation.

erties of the incoming light wave. Also, light in its turn affects the liquid crystal. This feedback between light and the liquid crystal gives rise to a wide range of complex optical phenomena. Therefore, advanced numerical techniques are often required to model them.

In my thesis I developed a method that takes into account the coupling between light and liquid crystals and apply it to study interesting and novel phenomena exhibited by light interacting with liquid crystals. In the heart of my approach lies the Finite-Difference Time-Domain (FDTD) method.

My aim was to develop a method for solving the feedback problem self-consistently by combining equations for liquid crystals with the FDTD method. In this method the dynamical response of liquid crystals to optical fields is considered at the same time as changes in optical field due to interaction with liquid crystals. This new approach would allow the study of various nonlinear phenomena in liquid crystals, in particular when both the liquid crystals and the field response to each other are important.

In this paper I desribe how the method developed in my thesis can be applied to studying the interaction between a real laser beam and a liquid crystal medium.

This paper is arranged in the following way. First, in section 2 the basics of singular optics are discussed. Then, section 3 describes how a liqud crystal can induce changes in the laser beam. Section 4 demonstrates the birth of the vortex singularities. Finally, in section 5 I draw some conclusions.

Basics of singular optics

Singular optics is a relatively new area of optics, which studies the topology of wave fronts. In classical optics, wave fronts or surfaces of equal phases follow each other with a spatial separation of one wave length. However, sometimes for some reasons this separation can be violated due to local changes in phase velocity. This could lead to wave front collapse, where the phase of the wave becomes not defined and the amplitude is exactly zero. Points in space where this happens are called singular points.

Singularities of wave fronts were first mentioned in the connection with the tidal waves as described be Berry in [2]. In this paper it was found that tides move as gigantic waves. Lines of equal tide heights, also called co-tidal lines, are the lines of equal phases and thus the wave fronts of tidal waves. Figure 3 shows co-tidal lines distribution in the North Sea. Different lines correspond to different times. The two points where all the phase lines come together are places where it is high tide at all times, that is to say, no tide at all. These are the singularity points and in the theory of tides they are called *amphidromic points*.

One of the first observations of optical singularities was made be Zeldovich & Tabiryan in [4]. The peculiar appearance and disappearance of additional interference dark fringes were noticed in experiments where the laser beam that first passed though an optically nonlinear medium then interfered with the plane wave. Several explanations were proposed but the real breakthrough was made by Berry and Nye [5]. They introduced a new concept of phase singularities in the optical field as the new class of objects in wave theory. They also introduced the terms of *wave front dislo-*

Figure 3: The amphidromic points in the North sea represent the singularity in a tidal wave. Reproduced from [3].

cation in analogy with the theory of defects in crystals. According to them, wave dislocations are perfect interference fringes. They should not be confused with the dark fringes often discussed in elementary treatments of interference. These dark fringes are conceived as surfaces rather than lines, and defined as the places where two interfering waves are out of phase. This causes the intensity to be small, but it is only on the dislocation lines, where the two waves have equal amplitude as well as being in antiphase. This means that at the dislocation lines the intensity is exactly zero. Also, the wavefront dislocation is a more general concept, because it is applicable in cases where more than two waves interfere, or when two waves interfere with unequal or changing amplitudes.

Following Nye and Berry [6], let us show mathematically how the wave dislocations are born. The scalar optical field $U(x, y, z)$ can be described by a complex function:

$$U(x, y, z) = u(x, y, z) + iv(x, y, z) = A(x, y) \exp\{iS(x, y, z)\}, \tag{1}$$

where $A = \sqrt{u^2 + v^2}$ is the amplitude of the wave and $S = \arctan\{v/u\}$ is its phase. The wave front of the wave propagating along z-axis as the surface of equal phase is described by the following equation:

$$kz + \arctan\{v/u\} = \text{const} = 2\pi N, \tag{2}$$

where N is the front number.

At points in space $\{x, y, z\}$, where both $u(\{x, y, z\}) = 0$ and $v(\{x, y, z\}) = 0$, the function $\arctan\{v/u\}$ and thus the wave phase are not defined. Simultaneously, the amplitude A is equal to zero. The points $\{x, y, z\}$ therefore form dislocation lines and define the phase singularity trajectories. They are also called zero-lines.

The main topological property of a dislocation line is found by integrating the phase change on a circuit that encircles the dislocation line. It could be shown, that for a generic dislocation [6]

$$\oint S = 2\pi m, m = 0, \pm 1, \pm 2..., \tag{3}$$

where m is called the topological charge of dislocation strength. The deeper meaning of m will be explained later.

Thus one can formulate the main characteristics of the wave dislocation:

1. At the dislocation line both real and imaginary part of the optical field are equal to zero.

2. The phase of the wave at the singularity point is not defined and the amplitude is exactly zero.

3. The singularity can be described by the topological charge which is defined as the number of 2π jumps of the phase at the singularity.

The term dislocation is borrowed from crystallography, because wave dislocations interrupt the regularity of a system of wavefronts in precisely the same way that crystal dislocations disrupt a crystal lattice. By analogy, the classification of singularities is similar to the classification of the crystal defects. They can be pure edge, pure screw, mixed screw-edge, localized, nonlocalized and many more. Here, only one examples will be considered in more detail.

The analogue of the Burgers vector in crystals is a vector perpendicular to the wavefront of length equal to the wavelength. The pure screw dislocation is defined as this vector being parallel or antiparallel to the dislocation line. An example of a pure screw dislocation is the the exact solution of the wave equation U in the form:

$$U(x, y, z) = k(x + iy) \exp\{i(kz - \omega t)\}, \quad (k = \omega/c). \tag{4}$$

The wave front equation is given by:

$$kz + \arctan\{y/x\} = \text{const}. \tag{5}$$

Thus the surfaces of constant phase, $z = \arctan\{y/x\}/k + \text{const}$, the wavefronts, are helicoids with a pitch of one wavelength. At the point $x = 0, y = 0$ we observe screw dislocation of the wave front. This is the same as the crystal planes in a crystal containing a screw dislocation. As time progresses, the helicoids move in the z direction with velocity c. An example of the screw dislocation is given in Fig. 4. Here the phase of the wave is plotted and one can see that in the middle of the screw phase is not defined and jumps between the values. Screw dislocations are also known as optical vortices. The term optical vortices was first introduced in [12] by Coullet *et al* and it is in common use since then.

The next section describes singularities that appear in the wavefront of the light interacting with a liquid crystal and discusses a particularly important example of singularities formed by a Gaussian lens.

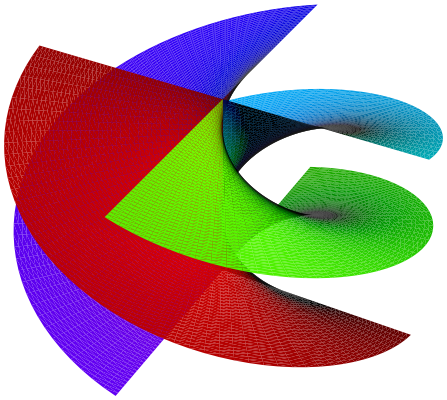


Figure 4: The screw dislocation - phase of the wave is undefined in the middle of the screw. Different colours correspond to different values of the phase. Picture courtesy of Mark Dennis [7].

Optical singularities induced by a liquid crystal medium

Liquid crystals are optically nonlinear media. This means that light passing through a liquid crystal slab changes the optical properties of the slab. This in turn affects the light propagation inside and outside the slab. For example, a liquid crystal-induced phase lag can lead to new wavefront properties. In particular, wavefronts that were smooth before interacting with the liquid crystal can become singular after the interaction. This phenomenon is called self-action and it makes liquid crystals very interesting for studying the natural birth of optical singularities.

Various theoretical and experimental studies have been conducted in order to study wavefront singularities after a liquid crystal, in particular by Soskin and colleagues in Kiev [8-9]. It was shown that two conditions must be satisfied for the phase singularities appearance after a liquid crystal cell. The first is that the refractive index modulation must create either focussing or defocussing lens like structure. The second condition is that the optical strength of this structure must exceed the certain threshold value.

Let us consider the most common case of illumination a liquid crystal cell with a Gaussian beam. The term Gaussian beam normally refers to a beam with a Gaussian intensity distribution in the plane perpendicular to beam's propagation direction. It important to note that a real laser beam is often not symmetric in the xy plane. Also, due to various interactions inside the cell, the director distribution can be not symmetric in the xy plane even if a beam is symmetric. Therefore, it is interesting to consider a full three dimensional case without the symmetry in respect to z axis.

Previous studies [9-11] suggested that the whole scenario of the singularity birth changes for a case of the asymmetric director distribution. It was shown, both experimentally [14] and theoretically [11] that the asymmetric beam has interesting optical

properties, in particular when interacting with liquid crystals. In was found that after this interaction, optical vortex singularities can be observed in the far field. All these studies used the paraxial approximation and the non self-consistent approach to investigate the phenomenon of optical vortices. In this paper, however, the FDTD self-consistent algorithm will be used to consider the problem. In the next section, I solve Maxwell's equations inside the liquid crystal directly using the developed FDTD code. Then the self-consistent algorithm is applied in order to take into account the feedback between the laser beam and changes in the director profile.

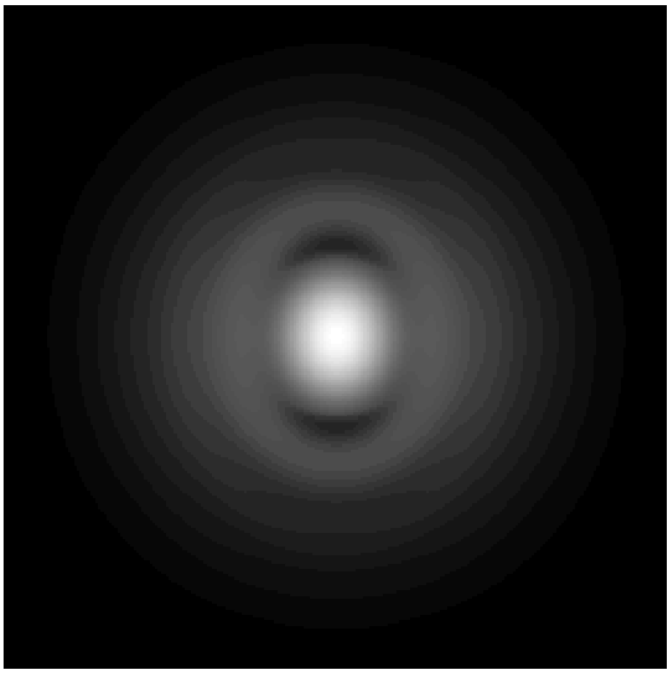
Observing optical vortices

In this section I show the results obtained by the self-consistent FDTD algorithm.

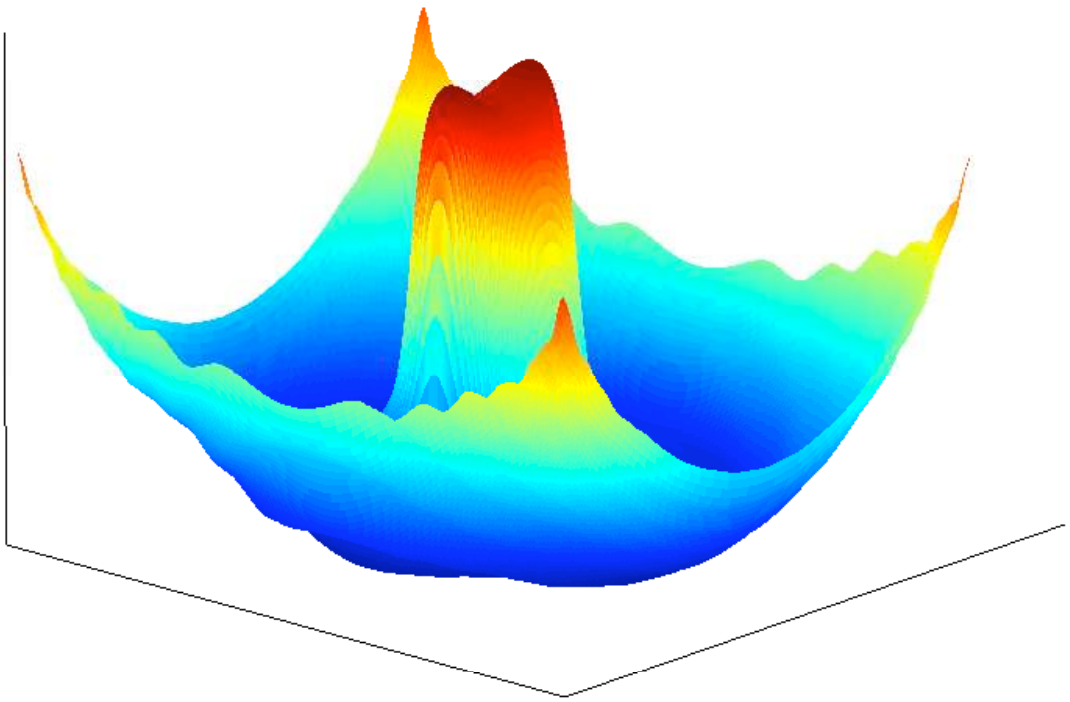
In Figs. 5a-9b the transformation of laser beam after the cell is shown. Figs. 5a-5b show the beam at $z = 0.09z_L, z_L = \pi L^2/\lambda$, where L is the width of a liquid crystal cell and λ is the light wavelength, just before the point where the first singularity is born. In Fig. 5a one can see two points where the amplitude is nearly zero. Fig. 5b shows the phase with a drop of nearly π. Increasing the distance increases further to $z = 0.1z_L$ sees the appearance of two side $\pm\pi$ jumps and the two point dislocations along x-axis are born and exist in the wavefront. This is shown in Figs. 6a-6b. By increasing the distance further, the beams begins to diverge. When it reaches $z = 0.16z_L$ one can see four optical vortices in Figs. 7a-7b. This is also called an optical quadrupole with alternating $+1$ and -1 charges in accordance with the sign principle of the enclosed system [13] and experimental observations [8]. Then the optical quadrupole reaches preannihilation stage at $z = 0.18z_L$. Fig. 8a shows how the zeros of amplitude are coming closer and nearly form two point dislocation again, this time it is orientation is along the y-axis. Fig. 8b shows the phase changes at this distance. Finally at $z = 0.21z_L$ the pronounced two points dislocation, now along the y-axis is observed in Figs.9a-9b. With increasing the distance from the cell, the singularity disappears and the phase is smooth again.

The scenario of optical singularities birth is thus as follows. First the optical dipole is observed along the axis that corresponds to smaller width of the incident beam ω_1. This dipole then splits into a quadrupole that moves around toward the other axis. Eventually it annihilates into a dipole along the axis that corresponds to the larger width of the incident beam ω_2.

It is also interesting to compare the pictures showing lines of constant phase for different distances after the cell. Fig. 10a shows the lines of constant phase at the exit from the cell. These lines reflect the Gaussian distribution of the phase. There is no circular symmetry as the incident beam is not symmetric. The lines are smooth corresponding to the smooth wavefront. Fig. 10b shows the lines of constant phase at the pre-dislocation stage. Here one can observe the appearance of the valley in the phase distribution shown in Fig. 5b. Fig. 10c shows the lines of constant phase at $z = 0.1z_L$, where the two-point singularity is born. Here one can observe the appearance of discontinuities in the lines, which corresponds to the jumps in the phase shown in Fig. 6b.

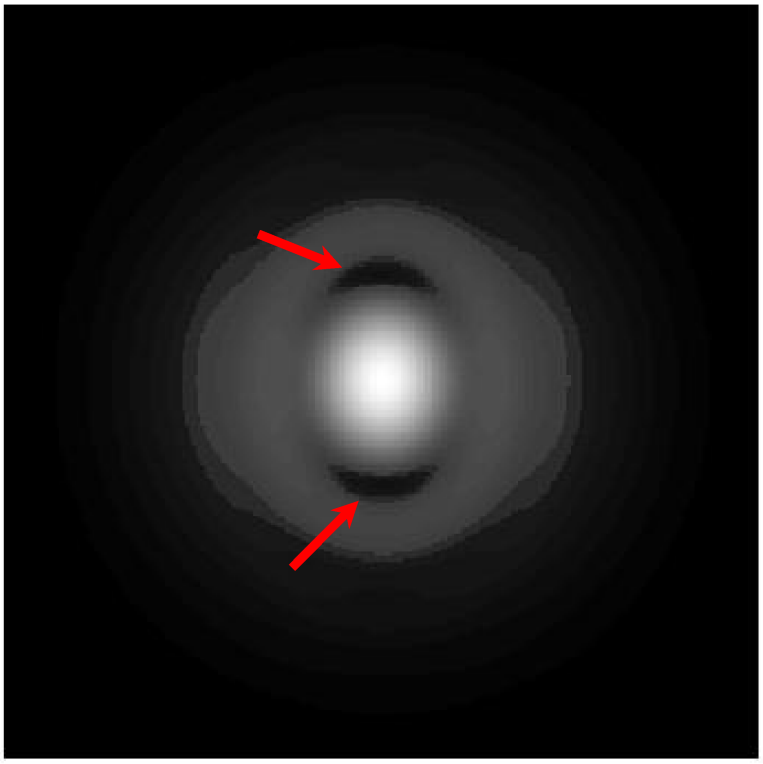


(a) Amplitude of the beam at the pre-dislocation stage.

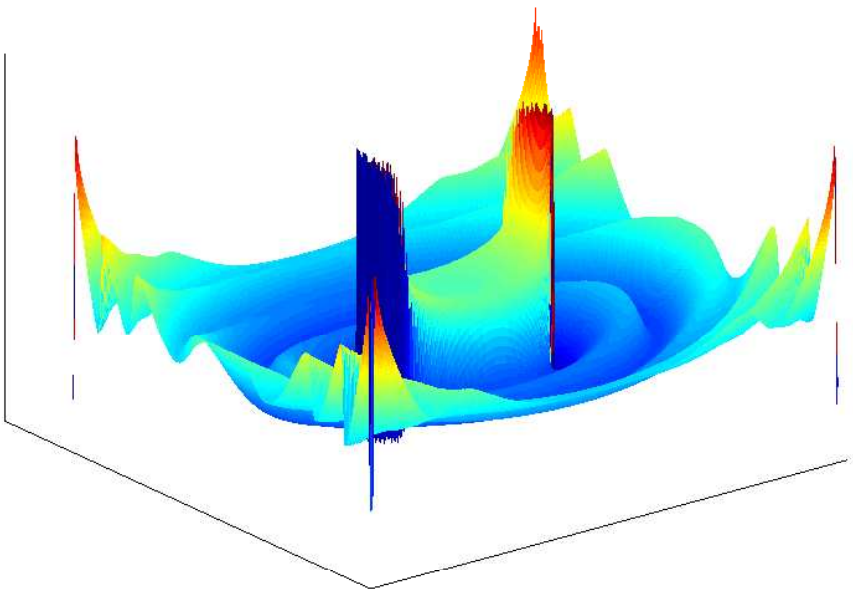


(b) Phase of the beam at the pre-dislocation stage.

Figure 5: Amplitude and phase of the beam at the pre-dislocation stage. $z = 0.09 z_L$.

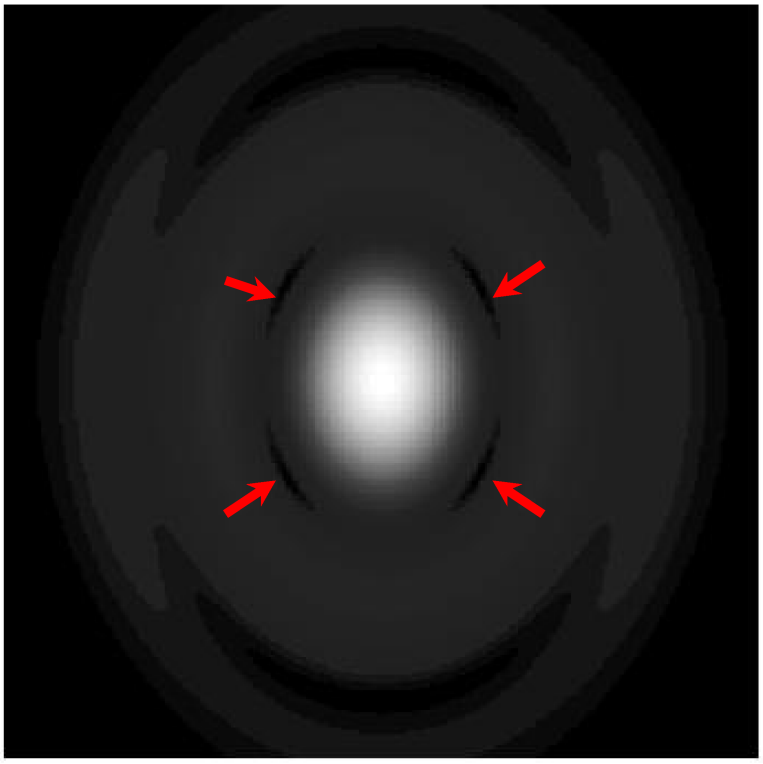


(a) Amplitude of the beam at $z = 0.1z_L$ - two point dislocation along x-axis (dipole) is born. The dislocation points are shown by arrows.

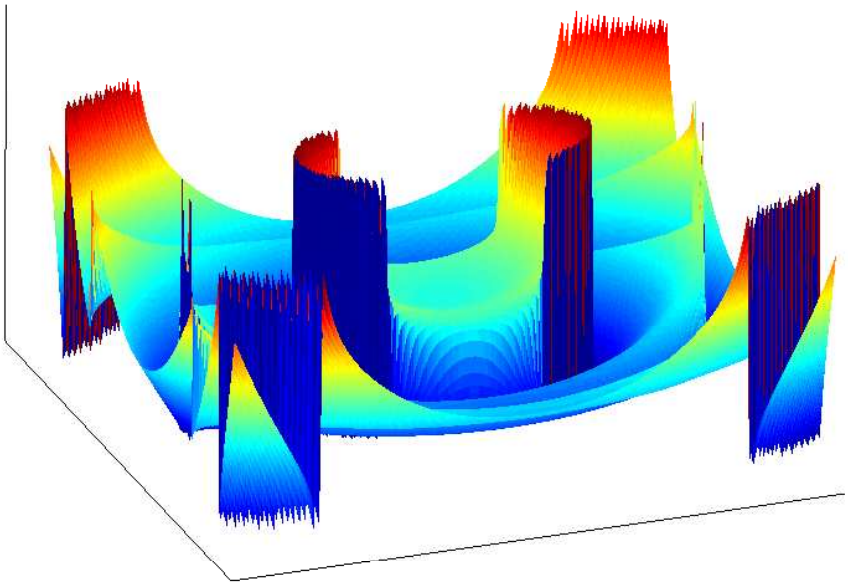


(b) Phase of the beam at $z = 0.1z_L$.

Figure 6: Amplitude and phase of the beam at $z = 0.1z_L$ - the two point dislocation along the x-axis is born.

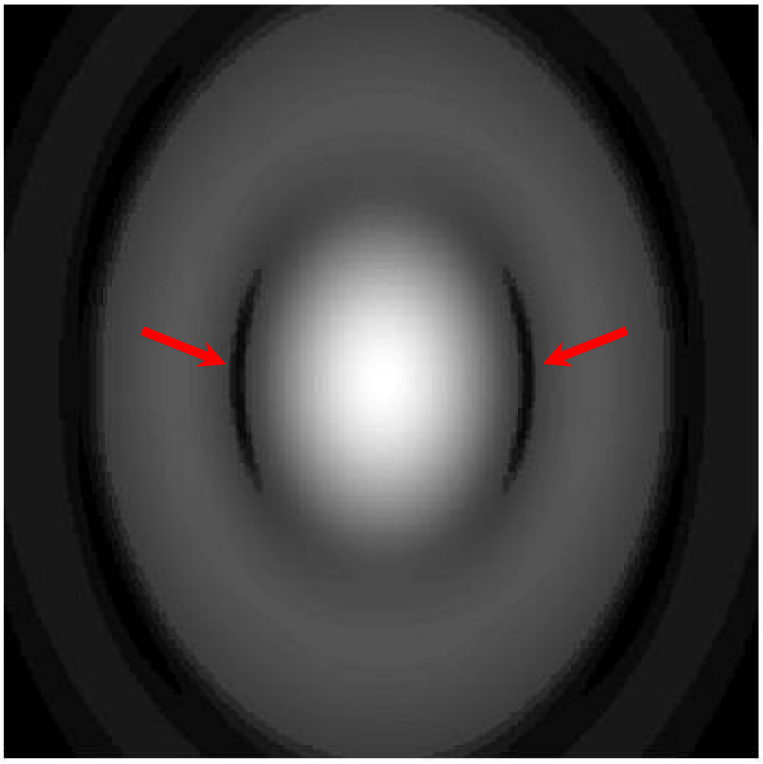


(a) Amplitude of the beam at $z = 0.16z_L$ - optical quadrupole. The dislocation points are shown by arrows.

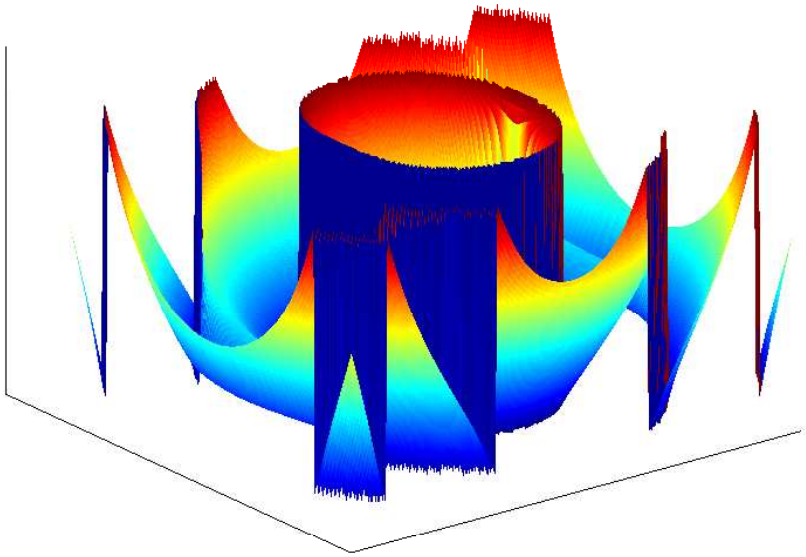


(b) Phase of the beam at $z = 0.16z_L$.

Figure 7: Amplitude and phase of the beam at $z = 0.16z_L$ - the optical quadrupole is born.

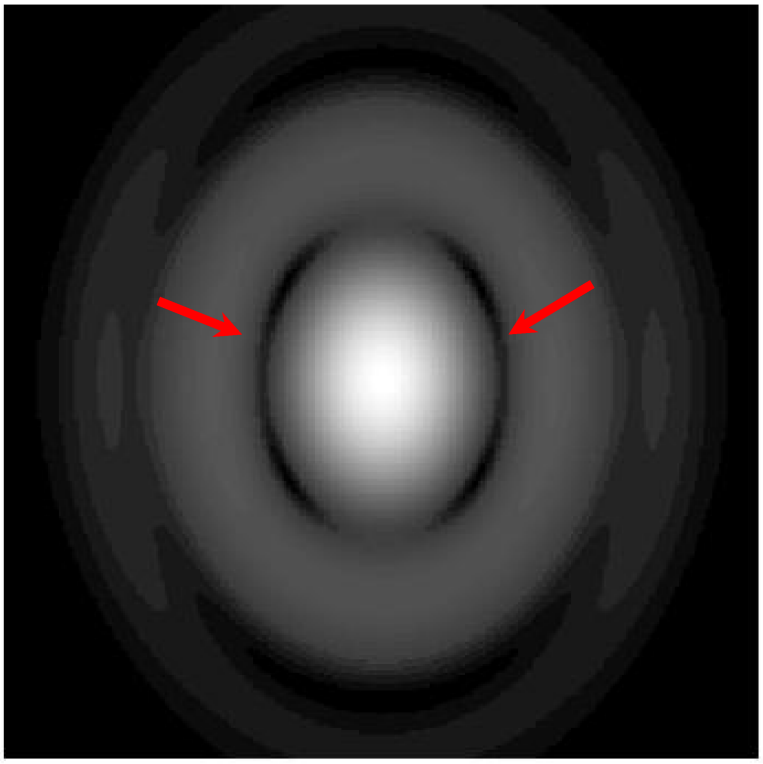


(a) Amplitude at $z = 0.18z_L$ - the optical quadrupole is about to annihilate into the dipole. The dislocation points are shown by arrows.

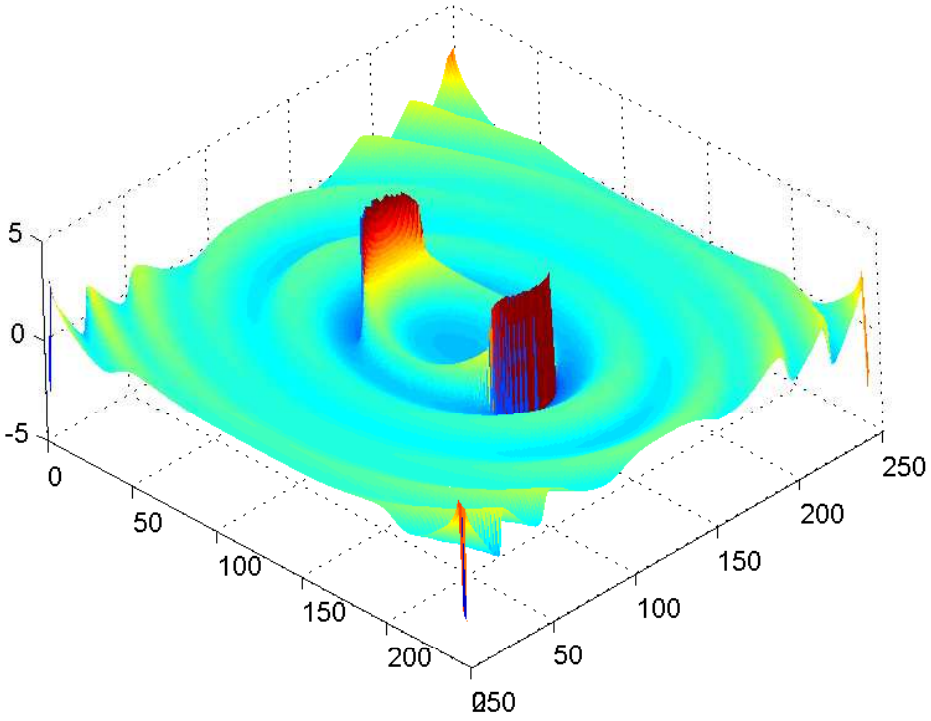


(b) Phase of the beam at $z = 0.18z_L$ - the optical quadrupole is about to annihilate into the dipole.

Figure 8: Amplitude and phase of the beam at $z = 0.18z_L$ - optical quadrupole is annihilating into the dipole with orientation along the y-axis.

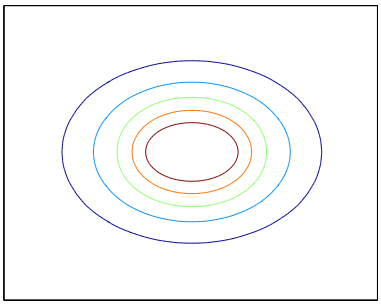


(a) Amplitude at $z = 0.21z_L$ - two point dislocation (dipole) along y-axis. The dislocation points are shown by arrows.

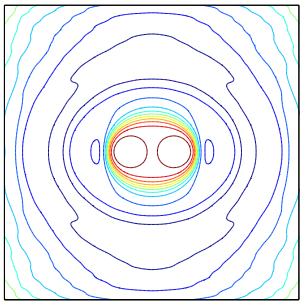


(b) Phase at $z = 0.21z_L$ - two point dislocation (dipole) along y-axis.

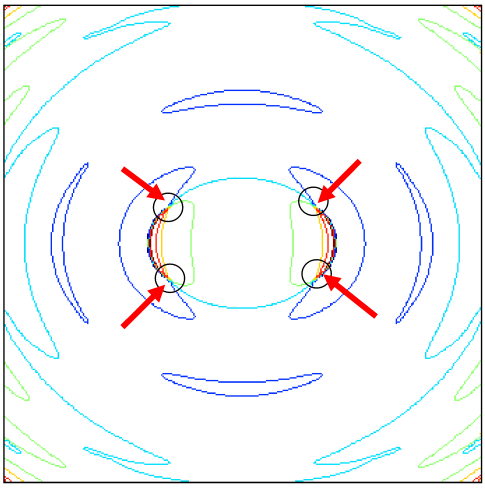
Figure 9: Amplitude and phase of the beam at $z = 0.21z_L$ - optical quadrupole has disappeared annihilating and the dipole with orientation along the y-axis is born.



(a) Lines of constant phase at the exit from the cell. Smooth lines reflect a smooth wavefront.



(b) Lines of constant phase at the pre-dislocation stage. The picture corresponds to the appearance of the valley in the phase distribution .



(c) Lines of constant phase at the dislocation distance. The singularities corresponding to the optical quadrupole are shown by circles and arrows.

Figure 10: Lines of constant phase at different distances from the cell.

Conclusions

In this paper I have analysed the astigmatic Gaussian beam interaction with a liquid crystal cell. The self-consistent algorithm together with the FDTD Maxwell solver have been used to study the problem.

The beam propagation beyond the cell is of particular interest. This is because previous studies suggest the appearance of different types of optical singularities in the wave front. They appear because of the liquid crystal nonlinear optical properties, which lead to birefringence and hence to local variations in the wave front speed of propagation. Thus the liquid crystal acts as a lens with a complex phase factor. In the case of a Gaussian incident beam this factor can be approximated with a Gaussian function and therefore a liquid crystal has a similar effect to a Gaussian lens on beam propagation.

Beyond the cell the beam focusses and then diverges again. This is the region where optical singularities are expected to appear. For astigmatic beam they are optical vortices that appear first as a dipole along one of the axis and then move to form an optical quadrupole. Further they move again to form a dipole along another axis.

These results confirm principal scenarios for the birth of the optical singularities that have been predicted by a different method. In work [9] the Gauss lens analogy was used to study scenario of singularities evolving. In [11] the author used paraxial approximation to describe the beam propagation inside the liquid crystal. However, the positions of singularities are different. The difference in results is due to more accurate calculation of the exiting field by the FDTD method and the director distribution in the self-consistent algorithm. The internal intensity is always smaller than incident intensity and so is the maximum distortion of the director. Thus the results are always shifted to lower intensities.

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Dr Vera Hazelwood is the winner of the IoP Computational Physics Group thesis price 2007. She is now working at the Smith Institute for Industrial Mathematics and System Engineering, and can be contacted at Vera.Hazelwood-at-smithinst.co.uk.

Computational Physics Group News

The Computational Physics Thesis Prize 2008

The Committee of the Institute of Physics Computational Group has endowed an annual thesis prize for the author of the PhD thesis that, in the opinion of the Committee, contributes most strongly to the advancement of Computational Physics. A total prize fund of up to $\pounds 250$ will be divided between the prize-winner and the runners up. The number of awards is at the discretion of the Committee. The winner(s) would be expected to provide an article for the IoP Computational Physics Group Newsletter.

- ▷ The deadline for applications is February 28^{th}, 2009.
- ▷ The submission format is a 4 page (A4) abstract (pdf) together with a citation (max. 500 words) from the PhD supervisor and a confidential report from the external thesis examiner. Further details may be requested from shortlisted candidates.
- ▷ The submission address is:
  DR NUNO LOUREIRO
  email: Nuno.Loureiro@ukaea.org.uk
- ▷ Please enclose full contact details, including an email address.

Applications are encouraged across the entire spectrum of Computational Physics. The competition is open to all students who have carried out their thesis work at a University in the United Kingdom or the Republic of Ireland, and whose PhD examination has taken place in 2008.

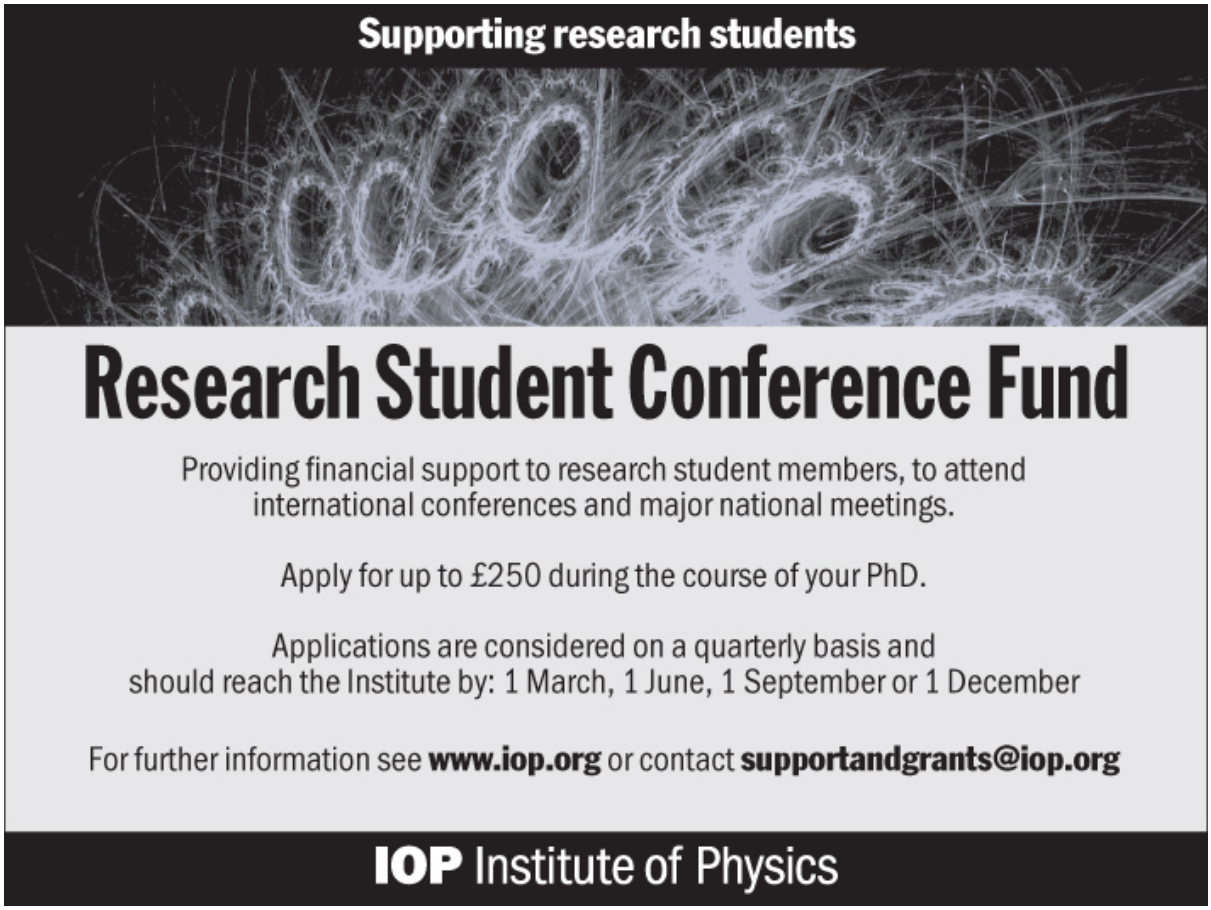
International Union of Pure and Applied Physics: Young Scientist Prize in Computational Physics

The "International Union of Pure and Applied Physics Young Scientist Prize in Computational Physics" (IUPAP Young Scientist Prize) can be awarded to researchers who have a maximum of 8 years research experience following their PhD.

See `http://c20.iupap.org/prizes.htm` for details.

IoP Computational Physics Group - Research Student Conference Fund

The Computational Physics Group (CPG) of the Institute of Physics (IoP) 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 can be found at

`http://www.iop.org/activity/grants/Research_Student_Conference_Fund/page_26535.html`

Reports on meetings

2008 APS March Meeting

New Orleans, Louisiana, USA, March 2008

The APS March Meeting at New Orleans was my first international conference with oral presentations about Theoretical study of melamine superstructures and their interaction with the Au(111) surface. I talked the self assembly of melamine on the Au(111) surface and the method applied to simulate such system.

The conference hall was very huge, and for me it was unbelievable that so many people can present so many works in different fields. The duration of each talk was very short (only ten minutes) plus two minutes for the questions. Sometimes it was really hard to understand the aim or the final results of the work done. Although the time was really short, there was no delay during the oral sessions. Moreover, there was a focus session every day which anyone can attend (for example, my talk was in the session Self-assembled organic overlayer). What was also very interesting is the poster session where a lot of different works were presented and where you can ask more questions compared to the oral session presentations.

My talk was appreciated by an experimental group that can lead to a future collaboration on better understanding of polymeric systems under different conditions.

Not all talks at the APS March Meeting were only ten minutes long. Invited talks were longer, which made them easier to understand. Moreover, there were special talks during the special session where very important people for the physics spoke about their past and actual work. I followed many talk interesting like the section Frontiers of computational materials or Fundamental Developments in Density Functional Theory.

This conference was not only organized to present talks and poster but also to present books, software packages and experimental instruments. There was software to make plots or package to look up for references. The most interesting was the book exhibition where anyone can find a book useful for own research field. In my field there were several books in computational and polymer physics.

This conference was very useful to understand where the research is going (not only in my field), what are the possibilities in the future and have one idea about the other physicist are doing. Such a big conference gives possibility to interact with a lot of different people that work in the same research field and allows for exchange of ideas. This will help to improve the work I am doing in my PhD project.

Manuela Mura, King's College London

Intermag 2008

Madrid, Spain, May 2008

The Intermag conference is considered to be the premier conference on applied magnetics and information storage technologies. Annually, it brings together members of the international scientific and engineering communities interested in recent developments in magnetics and associated technologies. I went to the Intermag conference in Madrid with a number of colleagues from York including many members of academic staff.

The conference was held at the Palacio Municipal de Congresos, an excellent building for conferences with modern architecture. On the Sunday evening, after our arrival, the conference registration began and I was able to meet many prominent workers in the field. This was followed by 3 invited talks about multiferroics materials. Later, after the finish of the talks I discussed with my colleagues the potentially interesting talks of the conference to come.

Monday morning, I attended the symposium about the interface and the transport properties of thin films as well as the heat and microwave assisted recording symposium where a member of our group was presenting a talk. On the evening, I went to the symposium on the importance of GMR. The talks of this symposium were discussing mostly historic facts and latest developments of GMR. After that the more celebrating part of the conference began in recognition of the Nobel Prize for the discovery of GMR. This year's Nobel Laureates in Physics, Prof. Albert Fert and Prof. Peter Grunberg, delivered lectures about GMR and beyond followed by Champaigne toasting.

As my field of research is the atomistic simulation of exchange bias systems, on the second day I decided to attend the sessions Exchange bias I and Magnetic Modelling. Talks on the dependence of exchange bias on antiferromagnetic thickness dilution and cooling process were very interesting and useful for comparison with my results. Also, very good talks were given from my colleagues in York presenting experimental results. On the second symposium, new methods of modelling were presented from numerous presenters. Much attention was drawn to a talk about modelling of nanoparticles with exchange bias effects given by Prof. O. Iglesias and a talk about new ways of modelling magnetic properties using the Wand-Landau method given by Prof. T.C. Schulthess. Later that day was the IEEE Magnetics society annual meeting were various matters were discussed considering the society organisation.

Wednesday morning was the time to present my poster in the Exchange bias II poster session. I had some interesting discussions with people of other universities (especially Taiwan) about the training effect of exchange bias and how these results are compared with their experimental findings. On the evening, I joined the very interesting and unusual symposium Life Science and applications II. Talks about the effect of magnetic field reversal on animals and especially in the orientation of pigeons were very interesting and funny. Later that day, there was an IEEE Magnetics Society Awards ceremony in which one of my supervisors was nominated fellow of the society. Also, the plenary session of the conference was given by Prof. Ludwig Schultz,

discussing magnetic levitation and its application to levitating trains, with an excellent real demonstration.

Thursday morning, we continued going to talks which looked interesting in the program booklet and visiting the poster sessions. There were a number of quite interesting posters about computational magnetism and micromagnetics. In the exhibition there were software companies presenting general software for magnetic or more general condensed mater simulations. During lunch time, I visited the Prado museum of fine art, an excellent opportunity to see paintings of El Greco and Goya. Finally, on the last symposium of conference I watched the talk of my colleague about modelling single antiferromagnetic grains in exchange bias systems.

I found the conference both very interesting and educational and I gained a significant benefit from its attendance. I am very thankful to the Institute of Physics Computational Physics Group for partially funding my attendance.

Andreas Biternas, Computational Magnetism Group, University of York

New Model and Hydrocodes for Shock Waves Processes in Condensed Matter Physics

Lisbon, Portugal, 18-23 May 2008

This was the seventh meeting of the bi-annual, international conference: New Models and Hydrocodes for Shock Wave Processes in Condensed Matter (NMH). The conference series brings together many people from many different countries, including Russia, USA, France, Germany, and the UK. There were nearly 100 talks presented in the sessions with most of the computational modelling being devoted to the afternoon. With so many good talks I heard, I can only pick out a few highlights of the conference.

A very interesting talk was given by Tim Germann of Los-Alamos National Laboratory (LANL) on shock induced particulate ejection using molecular dynamics with empirical potentials. Germann and co-workers simulations were performed on the LANL supercomputer BlueGene/L and contained a billion atoms. The simulations ran for between 24 and 48 hours on the whole of BlueGene/L (212,992 CPUs) which was the equivalent of running the simulation on 1 cpu for a millennium! Germann also discussed the new LANL supercomputer called Roadrunner which is currently being put together at IBM. It is expected that Roadrunner will top the peta-op calculation ability.

G.V. Ionov of the Russian Federal Nuclear Center gave an interesting talk on determining a crystal structure. In Ionovs talk, Adaptive Template Analysis of Crystal Structures and Defects in Molecular Dynamics Simulation of the High-Strain-Rate Behavior, he showed how his Adaptive Template Analysis (ATA) method could accurately and with little error recognise 4 different crystal structures - FCC, HCP, BCC and diamond on structures that had vacancies, interstitial atoms and dislocations.

My presentation was entitled Shock Wave Simulations of Alpha-Quartz and I spoke

about the calculation of high pressure phases in quartz after subjected it to an intense shock wave.

The above talks were all atomistic in nature, however this conference also contained many hydrodynamic talks. One that stood out was Andrew Barlows talk from The Atomic Weapons Establishment (AWE), entitled Extending Compatible Lagrangian Hydro to Multi-Material ALE followed on from his talk last conference on his work to extend AWEs Arbitrary Lagrangian Eulerian (ALE) code to incorporate a nite volume scheme. Much progress has been achieved.

The conference for me was very useful as I got to meet some great people in the eld and to get some new ideas for my own research. I think the conference was well worth attending!

Matthew Farrow, University of York

39th Annual Meeting of the Division of the Atomic, Molecular and Optical Physics

Pennsylvania, USA, May 2008

39th Annual Meeting of the Division of the Atomic, Molecular and Optical Physics

From the 27th to 31st May 2008 I attended the 39th conference meeting of the Division of Atomic, Molecular and Optical Physics (DAMOP) held in State College, Pennsylvania, partially funded through a grant awarded by the Institute of Physics (IOP). DAMOP represents a major annual USA conference of sufficient importance that IOP publishing has a regular presence.

The scientific portion of the meeting was launched with the DAMOP Prize Session, featuring presentations from Horst Schmidt-Bocking (Davisson-Germer Prize) and Kenneth Kulander (Allis Prize). Over 60 invited, focus, and contributed sessions had been scheduled over the next three and half days, a number of which were applicable to my own area of research, concerned with the calculation of accurate, high-quality atomic data using the general atomic structure code CIV3. Those which proved to be most beneficial included:

- ▷ Clocks, precision measurements and atomic/molecular structure.
- ▷ Focus session: atomic polarisation and dispersion, specifically talks detailing work on relativistic many-body calculations.
- ▷ Photoionisation and photodetachment processes.

A scientific talk elaborating on the development of a method designed for calculation of atomic properties, which combines the all-order procedure with the configuration interaction approach was of particular interest.

One of the special events organised was a tutorial session held by Physical Review A and Physical Review Letters, aimed at providing insight and advice relating to research publication, a topic which would appeal to the majority of researchers.

Our current work on neutral tin, which is required for a study of impurities in the new generation tokamaks, was presented among 431 posters at one of the three ar-

ranged poster sessions, entitled Atomic and Molecular Structure and Properties: Theory. As expected, these sessions afforded the opportunity for fruitful informal discussions on current atomic structure research with theorists from other institutions. Most notably, I had an enlightening conversation with a researcher from the National Institute of Standards and Technology regarding the implications of my own research as applied to the spectroscopic labelling of atomic energy levels. The work, undertaken with Prof. Alan Hibbert, involved the study of transitions in neutral chlorine, and was recently published in J Phys B 40 2847 (2007). Also, I briefly discussed the possible applications of our calculations on Sn I in collisional work with another member of the atomic physics community.

The next DAMOP meeting is scheduled for late May 2009 at the University of Virginia in Charlottesville, and I would encourage both theorists and experimentalists in related fields to attend this premier meeting in atomic, molecular and optical physics.

Paul Oliver, Queen's University Belfast

Molecular Dynamics for Non-Adiabatic Processes meeting

Institute of Physics, London, UK, 21/22 July 2008

- Day 1 Session 1: Transport at the nanoscale
  - Tchavdar Todorov: Correlated electron-ion dynamics in atomic wires
  - E. K. U. Gross: Time dependent density functional theory
  - Lev Kantorovitch: Nonequilibrium statistical mechanics of classical nuclei interacting with the quantum electron gas
  - Mads Brandbyge: DFT-NEGF approach to electron transport in nanoconductors: Vibrational signals and Joule heating
- Day 1 Session 2: Collision dynamics
  - Jonathan Tennyson: High accuracy first principles calculations of molecular spectra
  - Dorothy Duffy: Electronic Effects in Radiation Damage Simulations
  - Dan Mason: How good is damped molecular dynamics as a method to simulate radiation damage in metals?
- Day 2 Session 3: Molecular processes
  - Oleg Prezhdo: Dynamics at the nanoscale: Ab initio non-adiabatic molecular dynamics of quantum dots and carbon nanotubes
  - Sebastian Westenhoff: Resonant exciton energy transfer as a nanoscale measuring tool in conjugated polymers
  - Lorenzo Stella: A new approach to correlated electron-ion dynamics and its application to model nonadiabatic systems

Andrew Horsfield

Satellites and Computers

Institute of Physics, London, UK, 22 October 2008

Dr Craig Underwood, Deputy Director of Surrey Space Centre (SSC), talked about the challenges arising from ionising radiation and high magnetic fields.

Dr Trevor Dimbylow described the support of science operations on satellites carried out at the Space Science and Technology Department (SSTD) at the Rutherford and Appleton Laboratory (RAL).

Dr Phil Palmer (SSC) showed different methods of managing large assemblies of satellites using both ground control-to-satellite and satellite-to-satellite communication.

Finally Stuart Duncan, of Surrey Satellite Technology Ltd, described the very fine controls needed to keep GPS satellites in exactly the right attitude with respect to the Earth.

Roger Barrett

Selected Upcoming Computational Physics Events

Computer Simulation and the Environment

- ▷ Thursday, 10 September 2009
- ▷ Institute of Physics, London
- ▷ A one day meeting at which the first three speakers will talk about computer intensive modelling of physics related to the environment, followed by two presentations from hardware vendors on what the next generation of hardware will be like.
- ▷ Further information: http://www.iop.org/ConferencesSept2009

European Workshop on Monte Carlo Treatment Planning

19-21 October 2009, Cardiff, UK.

Conference on Computational Physics (CCP) 2009

16-19 December 2009, Kaohsiung, Taiwan

Computational Tools: LyX— LaTeX for the Word generation

Andrew Horsfield, Department of Materials, Imperial College London

Introduction

LaTeX has a well deserved reputation for producing high quality documents, especially those involving equations. Traditionally a document is typeset with a text editor, and for many people nothing else will do. Indeed a number of editors have a wide range of special features to assist with typesetting. This approach clearly has advantages if you are after total control over every detail, but it has downsides as well. While I believe that LaTeX is indeed the correct way to typeset scientific documents, I no longer use emacs to do this: instead I now (almost) always use LyX, and ask my students to do the same. Why? There are several compelling reasons in my opinion, which break down into three categories:

1. Ease of learning
2. Ease of use
3. New functionality

Let us look at these one at a time.

Ease of learning

Some like to dismiss Microsoft Word as some inferior, bloated, buggy product. I disagree. The road to its current status may not have been smooth, but the version we have today (included in MS Office 2007) is good. In particular, it is easy to use, is fast and reliable, and produces high quality output. Because almost everyone is familiar with it, it defines an effective standard for competing products. However, MS Word is not a natural tool for scientific document preparation: strict structuring is hard work to enforce; the basic equation editor is inadequate; citations are somewhat clumsy and require external software; figures have a will of their own. These deficiencies are absent from LaTeX. So, when new students arrive to work with me who are not familiar with traditional UNIX tools, but are familiar with MS Office, some appropriate response is needed. My answer is LyX. It is easy to use: the graphical interface is now really quite intuitive, and it is not hard to learn how to produce simple documents possessing the full beauty of LaTeX. Even typesetting equations using the menu bars is straightforward. The interface may not yet be quite as polished as MS Office 2007, but it is really quite good, is getting better all the time, and it gives you access to important functionality missing from Word.

Ease of use

But LyX is not just a set of training wheels for newcomers to LaTeX: I believe it has much to offer experienced users as well. The equation editor is superb. If you are familiar with LaTeX commands, then you just type them as you would in your favourite text editor, and you will see the equation building in front of you. I find this eliminates many frustrating errors. If you cannot remember the markup for a particular symbol, there is the option to use the extended toolbars to locate the symbol you want, which saves digging through books or web pages. The new dialogue for setting up the document allows very easy reformatting of the entire document (including margins, fonts and paper size). And if you use tables then the graphical table builder makes life much easier.

New functionality

LyX also includes new functionality that is not easy to capture with a text editor. The one that you are likely to come across first is the system for managing cross-references within a document (for referencing equations, figures, sections etc.). Both adding labels and referencing them has been made simple. Next up is probably the citation manager for the bibliography. This works with a BibTeX file, and is once again easy to use. But maybe the "killer application" is change tracking. This works in the same way as in Word (or OpenOffice) and is a great help when collaborating on writing papers. Of course, this requires all the collaborators to use LyX.

Conclusion

I hope I have given you some reasons at least to look at LyX. It is a well maintained program that just keeps getting better, and is available for Windows, UNIX/Linux and Mac OS X platforms. If you want to learn more, you can download it from `http://www.lyx.org/`. Enjoy.

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IoP Computational Physics Group links:

- ▷ Group webpages (http://www.iop.org/activity/groups/subject/comp)
- ▷ Newsletters (http://www.soton.ac.uk/~fangohr/iop_cpg.html)

Comments about the newsletter, letters and contributions for future editions are welcome and can be sent to Hans Fangohr.