An actual LHC collision event detected by the ATLAS detector and (inset) a Monte-Carlo representation of such a collision event
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**Computational Physics Group Committee**

**Related newsletters and useful websites**
Dear Readers,

In this Autumn 2011 edition of the newsletter, the feature article and cover image is an invited contribution from Dr Frank Siegert who has won the 2010 PhD Thesis prize awarded annually by the Computational Physics Group.

Please note that the newsletters for the last 2 years can be found online at:

Old editions of the newsletter can also be found online at:
www.soton.ac.uk/ fangohr/iop_cpg.html

Most URLs mentioned in the newsletters have hyperlinks and clicking on them should take you to the corresponding page. As always, we value your feedback and any suggestions for contributions in future editions. Please email the newsletter editor David Shipley (david.shipley@npl.co.uk)

The Computational Physics Group Committee.

The Computational Physics PhD Thesis Prize 2010

The winner of the Computational Physics PhD Thesis Prize 2010 is Dr Frank Siegert for his recent work on 'Monte-Carlo event simulation for the Large Hadron Collider' at CERN. His work is described below in the feature article of this edition. Frank's work was supported by a PhD stipend from the MCnet Marie Curie Research Training Network (contract number MRTN-CT-2006-035606).

Congratulations Frank!
Monte-Carlo event simulation for the Large Hadron Collider

Dr Frank Siegert, University Of Freiburg, Friburg, Germany, frank.siegert@cern.ch

Introduction

Much attention from physicists and the public has recently been focused on the subject of particle physics due to the start-up of one of its flagship projects, the Large Hadron Collider (LHC). Its goal is the study of fundamental particles and their interactions and currently most measurements in this area have come from high-energy particle colliders. The four experiments at the electron-positron collider LEP and two collaborations at the electron-proton collider HERA have finished their data taking a few years ago, while the Tevatron experiments will be continuing to deliver precise results from proton-antiproton collision data which was taken until September 2011. A new frontier has been reached in 2010 when the LHC at CERN started colliding proton beams at a new highest energy of 7 TeV and first measurements from several of its experiments were published.

Unveiling the mechanism of electro-weak symmetry breaking in the Standard Model (SM) has been one primary goal of many experiments. The Standard Model is a highly successful gauge theory so far and only one constituent of it, a fundamental massive scalar particle – the Higgs boson, has yet to be detected. Without this ingredient, the mechanism with which other particles acquire mass remains unexplained. Even despite the large success with which the Standard Model has made precision predictions for experimental measurements there are hints that it is not a completely fundamental theory. It contains 19 free parameters which can not be explained further from first principles, and it covers only three of the four fundamental forces, excluding gravity. Furthermore the so-called hierarchy problem poses the question, how the Higgs mass can be small enough to give the observed masses of the W and Z bosons. But also from an experimental point of view certain inconsistencies are starting to appear. Neutrino oscillations have been observed and contradict massless neutrinos as postulated in the Standard Model. There is also no viable candidate particle explaining the cosmological dark matter observations. Such considerations have spurred the interest in theories beyond the Standard Model.

It is the foremost objective of experimental particle physics to probe new theories by making measurements which might contradict Standard Model predictions. One of the tricky bits when trying to make such a claim is the smallness of the effects expected by the introduction of new theories. This requires very precise calculations of the prediction not only in the new theory, but also in the dominating Standard Model “background”. A big complication in that respect is the nature of Quantum Chromodynamics (QCD), which is part of the SM. Being a non-Abelian gauge theory with a massless gauge boson, QCD brings with it the property of asymptotic freedom: Its coupling constant becomes large at small scales leading to the confinement of its quanta into hadrons. Only at large scales can these partons be treated as free particles, allowing the application of perturbation theory. Perturbative calculations at large scales and their connection to the hadronisation scale together with a modelling of the confinement process all pose separate challenges which have to be overcome to make predictions for hadron colliders.

One tool to make predictions for collision experiments taking into account all aspects of QCD are Monte-Carlo (MC) event generator programs. Their most important feature is the ability to generate results at hadron level by the simulation of full events as they could then be observed by a detector. An “event” in this context is a collection of particle flavours and their momenta, which were created by the inelastic proton-proton-collision. Ideally, these simulated events are statistically a replica of the events generated by nature at the LHC such that kinematical distributions can be compared between simulation (theory) and measurement (experiment).

The availability of such fully exclusive events allows to study the effect of experimental techniques on signal and background directly. It also makes it possible for experimentalists to assess the impact of detector effects with the help of a dedicated detector simulation program and correct for them in their measurements. Ideally, and as practised recently in many experimental collaborations, this leads to the presentation...
of experimental results at the particle (hadron) level, which has a large advantage over both alternative options: If results are presented at the detector level it becomes difficult, if not impossible to interpret them from a pure particle physics point of view without knowledge of the detector hardware. In the other extreme, if experimental results are corrected to the parton level using some kind of model e.g. for any non-perturbative QCD effects, they become model-dependent, making them subject to the uncertainties of that model and also unfit for the further study of any new models.

**Parton showers and tree-level matrix-element corrections**

The most prominent examples of event generators are the highly successful, well-established programs HERWIG [1] and PYTHIA [2]. They have been constructed over the past decades alongside experimental discoveries and most of the features visible in past and present experiments can be described by them. In the last years though, in the run-up to the LHC, the development of Monte-Carlo generators has increased rapidly. There were mainly two reasons for such an effort.

From a technical point of view it became desirable, for maintaining as well as extending the codes, to use an object-oriented language (C++) and a modular design of the programs. This led to improved re-implementations in form of HERWIG++ [3] and PYTHIA 8 [4] – the successors of the Fortran versions mentioned above.

But more importantly, the large phase space available at LHC energies leads to a large amount of QCD bremsstrahlung from “colour charged” intermediate particles, analogous to QED bremsstrahlung (photons) from electrically charged particles. Since the coupling constant of QCD is roughly a factor of 10 higher than in QED, these effects play an even bigger role. Thus one obtains large rates for the production of multiple QCD partons at the LHC in association with other particles, e.g. $W$ or $Z$ bosons, $t\bar{t}$ pairs, boson pairs or photons. To calculate these rates it would be necessary to (automatically) draw and calculate all Feynman graphs which can connect the given initial and final states. One can imagine that this procedure becomes cumbersome and even unfeasible for a large number of partons.

Most of the radiation will be low-energetic gluons and quarks though which can be treated in an approximation allowing to take into account arbitrarily many such emissions. This can be illustrated for the first emission: Instead of calculating the full emission rate $R$ for a final state including one additional parton, one factorises it into the following pieces:

$$R \rightarrow B \times \left( \sum_{i,j} 8\pi\alpha_s \frac{1}{2p_ip_j} K_{ij}(p_i, p_j) \right)$$

- $B$ “Born” rate for the process without additional parton
- Sum over sub-terms $i, j$ of the factorisation, e.g. parton lines (DGLAP)
- $8\pi\alpha_s$ coupling constant
- $\frac{1}{2p_ip_j}$ massless propagator factor
- Universal $K_{ij}$ splitting kernel for branching $(ij) \rightarrow i + j$
  Specific form depends on scheme of the factorisation, but is independent of $B$

The factor in large brackets then represents the branching of one initial/final state parton into two and can be iterated to produce a “parton-shower” cascade, which is the main ingredient of the traditional MC event generators mentioned above.

Often it is not only this low-energetic region of parton production which becomes relevant though, but one needs precise predictions for the production of high-energetic partons. Here the parton shower approximation described above breaks down. It becomes necessary to supplement it with higher-order matrix-element corrections, calculated e.g. using Feynman graphs. One such approach, the correction of the
radiation pattern of the shower with higher-order tree-level matrix elements to as many orders as still feasible (ME+PS) [5], has lead to the development of the new multi-purpose Monte-Carlo event generator SHERPA [7]. The first part of my thesis deals with the extension of SHERPA in the simulation of perturbative QCD.

The ME+PS formalism based on the efficient replacement of splitting kernels in the parton-shower approximation with exact ratios of higher-order QCD tree-level matrix elements has been rewritten and significantly improved [6]. The main idea here is to apply a phase-space slicing with respect to QCD emissions by a measure related to the divergence structure of QCD. In the high-energetic emission region the parton shower is vetoed. This leads to a rejection of events, which will be compensated by adding events simulated using the exact emission matrix element. The formulation and implementation of this approach was done such as to preserve the resummation properties of the parton shower as well as the accuracy of the matrix element in their respective phase space regions. The success can be seen in Figure 1 where the phase space slicing criterion $Q_{\text{cut}}$ has been varied in a wide range. The two observables $d_{01}$ and $d_{12}$ are a measure of the emission rate in the first ($0 \rightarrow 1$) and second ($1 \rightarrow 2$) emissions and should be very sensitive to this kind of variation. With differences of only $\approx 10\%$ the algorithm is working very well.

![Figure 1: Study of ME+PS systematical uncertainties.](image)

The ME+PS algorithm has also been applied to the case of QED emissions for the first time in [8]. Internal consistency checks and a comparison to experimental data exemplify the performance of the algorithm. As a representative, Figure 2 displays a comparison of the new algorithm to data from the DØ experiment, showing excellent agreement also in the ratios between the measurement in different regions of phase space.

### Improvements for next-to-leading order accuracy

In the last section, the ME+PS idea was briefly summarised and it was argued that it allows to reinstate leading-order matrix-element accuracy into Monte-Carlo programs. At the same time it has to be made explicit that the inclusive rate of samples produced in such a way is still at leading-order accuracy only. Many matrix-element calculations on the other hand have already provided results at next-to-leading (NLO) or even next-to-next-to-leading order (NNLO) accuracy. Those go beyond the tree-level matrix elements by including also so-called virtual corrections initiated by Feynman diagrams with one or two loops respectively. There has been a number of proposals of how to include at least the full NLO results in a
Figure 2: Transverse momentum of the photon in $\gamma +$ jet events compared to measurements by DØ [9].

The differential cross sections and their ratios are displayed for four different regions of phase space, and have been scaled by factors of 5, 1, 0.3 and 0.1 respectively from top to bottom for better readability in the upper plot.
parton-shower simulation. However only two of them have been fully worked out and implemented in publicly available programs.

The first method, MC@NLO, pioneered in [10] and implemented for a large number of processes relies on using the parton-shower kernels and their universal soft and collinear properties to subtract the infra-red divergences of the real contribution to the NLO cross section. The subsequent parton shower then starts from either a Born-like configuration or from a configuration determined by the residual real correction contribution of the NLO calculation. By construction, there is some dependence on the details of the actual shower algorithm, which, to a certain extent, up to now seemed to limit the versatility of the method.

This dependence was overcome by the second method, POWHEG, which was initially presented in [11]. This technique essentially is an improvement of a re-weighting method which has been known for nearly two decades and was applied individually to a plethora of processes. To promote it to full NLO accuracy, it was supplemented with a local, phase-space dependent $K$-factor. Also the POWHEG method has been worked out for a number of processes in the framework of different parton-shower algorithms. A framework incorporating the core technology, independent of the specific parton-shower implementation and the matrix elements for the processes in question has been published in [12].

As a part of my thesis, the POWHEG method was implemented in SHERPA in an automated manner such that only the one-loop matrix element expression has to be calculated/interfaced on a per-process basis. All remaining pieces necessary for the calculation are available within SHERPA. Its performance is shown in the comparison to data for the transverse momentum and rapidity of the $Z$ boson in Drell-Yan lepton-pair production at the Tevatron in Figure 3.

![Figure 3: Transverse momentum and rapidity of the $Z$ boson in Drell-Yan lepton-pair production at the Tevatron compared to data from the DØ experiment [14,15].](image)

Both of these methods, POWHEG and MC@NLO, for matching of the parton-shower with NLO matrix elements have one deficiency with respect to the ME+PS method: They only include matrix-element corrections for the first emission on top of an inclusive process. Having at hand two, somewhat orthogonal, methods (ME+PS and POWHEG) to improve both the hard QCD radiation activity and the total event rate in a given process, the question naturally arises whether it is possible to combine both into an even more powerful approach. This was addressed by my thesis, resulting in a practical algorithm for merging both techniques. It has again been directly implemented into SHERPA and has meanwhile been made publicly available as open source software. In a parallel development, Hamilton and Nason [13] suggested an identical method; however, their actual implementation only approximates the formal result. Due to the formal equivalence of both proposals, they are generally referred to as the ME+PS approach.

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Only with such a combination does it become possible to get the inclusive cross section of a process accurate to NLO and at the same time correctly generate higher-order contributions according to their tree-level matrix elements. Measurements of the jet multiplicity in Drell-Yan events as well as the azimuthal angle between $Z$ boson and leading jet are highly sensitive to such higher-order contributions and are described very well with the MENLOPS approach in Figure 4. As can be seen, the POWHEG method alone does not reproduce the shape of these distributions well, and the ME+PS method has to be supplemented with a global $K$-factor to predict the inclusive rate of this process correctly.

Figure 4: Inclusive jet multiplicity (left) [16] and azimuthal separation of the boson and the leading jet (right) [17] in Drell-Yan lepton-pair production at the Tevatron.

Non-perturbative aspects of event generators

The last part of my thesis deals with the improvement of models for the non-perturbative parts of each collision event and was done in the context of the MC group of the ATLAS experiment at the LHC. Non-perturbative, unlike perturbative, QCD predictions can not be derived from first principles. Thus it was unclear before the start of the LHC how e.g. an existing model for multiple parton interactions would cope with the large jump in centre of mass energy of the collisions. An energy extrapolation was built into the model, but so far it had only been tested in the relatively low range from 630 GeV to 1960 GeV. A very quick comparison with early measurements at 7 TeV was thus eagerly awaited and the adjustment of the involved parameters became necessary to allow for a good estimate of the non-perturbative effects in future LHC simulations. To that end the non-perturbative parameters of the PYTHIA event generator are tuned using early measurements from ATLAS. It has to be stressed that the simultaneous tuning of multiple parameters to several measurements from different experiments is a challenging exercise. Three steps are involved in this procedure: First, predictions for each measurement are obtained by running the generator in many randomly selected configurations of the multi-dimensional parameter space. Second, the predictions are interpolated to the full parameter space. Third, using the interpolations, the minimum of the $\chi^2$ distribution based on the difference between interpolation and measured data in each bin of the observables is determined. In the case presented here, 7 PYTHIA parameters have been tuned to data from ATLAS, CDF and DØ at $\sqrt{s} = 0.63, 0.9, 1.8, 1.96,$ and 7 TeV. This constitutes the first comprehensive tuning of a MC event generator to LHC data. The results obtained with the new tune (dubbed “AMBT1”), especially
in very inclusive measurements from ATLAS as displayed in Figure 5 show the improvement with respect to other existing tunes.

**Figure 5:** Comparison of the new AMBT1 tune to ATLAS minimum bias distributions [18].

**Conclusions**

Several state-of-the-art methods for the improvement of Monte-Carlo parton showers have been presented. Their common aim is the correction of hard/wide-angle radiation patterns using exact matrix elements while leaving the logarithmic accuracy of the parton shower intact. The approach of tree-level ME+PS merging has been revisited and significantly improved to formally preserve the logarithmic accuracy provided by the parton shower in both initial and final state radiation. These formal improvements greatly reduce the uncertainties induced by the merging procedure compared to previously employed methods. This statement holds for inclusive quantities such as total cross sections and jet rates, as well as for differential distributions.

For the first time, QED emissions have been consistently incorporated into the ME+PS merging algorithm...
using parton showers with interleaved QCD+QED evolution. This achievement allows a study of hard photon production including the effect of the fragmentation component, which is otherwise very difficult to generate with a parton shower. Comparisons to Tevatron data show very good agreement and major improvements with respect to other theoretical approaches based either on fixed-order calculations or a pure parton shower.

While ME+PS merging has been shown to be well capable of predicting higher-order corrections to the shape of observables it still only provides a leading-order prediction for the inclusive cross section. Another approach, the POWHEG method, aims at correcting a parton-shower Monte Carlo to full NLO accuracy in the inclusive cross section as well as the radiation pattern of the first emission. An implementation of the POWHEG algorithm into the SHERPA event generator was reported. It is worth stressing that this is the first time that the POWHEG method has been fully automated and applied simultaneously to various higher-order calculations using Catani-Seymour dipole terms for partitioning the real-emission phase space. Additional processes are easily added by merely linking the corresponding code for the virtual correction terms. Finally, improvements of non-perturbative models using early ATLAS data were discussed. Work within the MC group of the ATLAS experiment resulted in the first comprehensive tuning of an event generator to minimum bias measurements at LHC energies.

References


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[16] V. M. Abazov et al., DØ collaboration, Measurement of the ratios of the $Z/\gamma^* + \geq n$ jet production cross sections to the total inclusive $Z/\gamma^*$ cross section in $p\bar{p}$ collisions at $\sqrt{s}=1.96$ TeV, Phys. Lett. B658 (2008), 112–119, [hep-ex/0608052].


Computational Physics Group News

- **The Computational Physics Thesis Prize 2011**
  The Committee of the Institute of Physics Computational Group offers an annual 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 prize of £250 will be awarded to the winner.

  **Eligibility and deadline:**
  - Applications are encouraged across the entire spectrum of Computational Physics.
  - The competition is open to all students from a UK institution, whose PhD examination has taken place in 2011.
  - The submission deadline is **30th April 2012**.

  **Submission format:**
  - A four page (A4) abstract.
  - A citation from the PhD supervisor (up to one A4 page).
  - A confidential report from the external thesis examiner (up to one A4 page).

  Please enclose all contact details including an email address as further details may be requested from shortlisted candidates.

  **Submission Address (and for further details):**
  Dr Vera Hazelwood, KTN for Industrial Mathematics, vera.hazelwood@smithinst.co.uk

- **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](http://www.iop.org/about/grants/research_student/page_38808.html)
Conference and Workshop reports

• **DPG and combined DPG Spring Meeting 2011**

75th Annual Meeting of the DPG and combined DPG Spring Meeting 2011
13-18 March 2011, Dresden, Germany

This six day long conference held jointly by the German physical society's Condensed Matter, Atomic, Molecular, Plasma Physics and Quantum Optics groups this year attracted more than 7000 researchers and students.

The program was very extensive with roughly 40 sessions being held per day (running in parallel) each with roughly 10 oral presentations and poster session were held at lunchtimes and in the evenings. I particularly recommend the poster sessions as the conference organisers provided free draught German lager and pretzels for the duration.

There were dedicated computational physics sessions and the highlight of the conference for me was a talk in the GPU computing focus session in the Dynamics and Statistical-Physics session. Tobias Kramer from the University of Regensburg, Germany and Harvard University, Massachusetts, USA presented a first principle simulation of thousands of interacting electrons propagating across a bulk semiconductor device (Hall bar) to investigate the necessary conditions required to form a hall potential. This interacting many-body system has been efficiently implemented on a GPU in a desktop computer system.

In many respects the conference was a success and the organization of such a huge event was phenomenal. All participants were very friendly and many enjoyed speaking to a English attendee to brush up on their English before giving their talks (that coincidently have to be in English). The only downside of the whole conference was that a minority of session chairs took it upon themselves to re-arrange the order of some talks or even move them forward to suit their own needs with obvious backlashes!

*Report from Sebastian Pinski, University of Warwick*

• **Student Conference on Complexity Science 2011**

5-6 August 2011, University of Winchester, UK
Website: [server7.web-mania.com/users/NcckukLe](server7.web-mania.com/users/NcckukLe)

The first annual Student Conference on Complexity Science was held at the University of Winchester, UK on the 5th and 6th of August 2011. The event was jointly organised by PhD students from Doctoral Training Centres at the universities of Bristol, Southampton and Warwick and was attended by over 110 delegates - 80 of whom presented posters or oral presentations.

The EPSRC funded Doctoral Training Centres were set up to investigate issues relating to complexity science, a field which uses computational modelling and simulation to investigate the mechanisms giving rise to observable trends seen in fields such as social science and economics, climate and earth science, biomedical and neural systems, physical systems and materials science and many more. Accordingly students presented their work on a range of topics and were able to receive valuable feedback and suggestions from their peers.

Prizes were awarded to Maximilian Albert from the University of Southampton for his presentation on 'Domain wall motion in magnetic nanowires with edge roughness' and Maike Sonnewald, also from the University of Southampton, for her poster on 'Using entropy production to parameterise earth system heat transport'.

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[www.iop.org/activity/groups/subject/comp/](www.iop.org/activity/groups/subject/comp/)  david.shipley@npl.co.uk
Keynote speakers, whose travel and accommodation was generously sponsored by the Institute of Physics’ Computational Physics Group, were Lord Robert May, former president of the Royal Society and former Chief Government Scientist, and Professor Luis Amaral, Professor of Chemical and Biological Engineering at Northwestern University, Illinois. Lord May presented a discussion on using financial systems modelling to predict banking crises and Professor Amaral described how complexity science can aide management of medical care. Both keynote speakers also joined a careers question and answer panel along with five other accomplished professionals applying complexity science in both academia and industry. The conference also featured a number of networking events designed to facilitate communication and collaboration between PhD students.

Report from James Snowden

- European Medical Physics and Engineering Conference (EMPEC) 2011

Modelling and Simulation scientific meeting at EMPEC 2011
2 September 2011, Dublin, Ireland

The European Medical Physics and Engineering Conference was held from the 1st to the 3rd of September 2011 in Dublin, Ireland. The meeting was hosted by the Irish Association of Physicist in Medicine (IAPM). Trinity College welcomed over 500 delegates from all over the world. An extensive program was offered covering the main areas of interest in Medical Physics and Engineering from Radiation Oncology to Biomechanics and Rehabilitation Engineering. A large number of dissertations were presented over the three days divided in parallel sessions. Posters were available for viewing at the exhibition room at all times.

The Modeling and Simulation in Medicine sessions took place on the second and third days of the conference. They involved a total of nine oral presentations and sessions were well attended. The first session contained three 30-minute presentations, mostly dedicated to patient modeling. Tooley reviewed patient simulators during his presentation and Baker explained the importance of modeling tumour control, as a means of reducing complication risks. At the end of the session, Spize offered an intensive study of radiation transport in image guided radiotherapy. The second session comprised six oral presentations and the topic of interest was the Monte Carlo method. Dissertations discussed different applications of this method. Zhang and Veloza employed the Monte Carlo method to model beam filtration and simulation of a head and neck phantom in computed tomography, respectively. Sakellaris introduced a newly developed Monte Carlo model on simulating digital mammography.
Cranmer-Sargison gave a very interesting talk on diode detector modeling for small fields in MV photon dosimetry. He highlighted that measuring output factors for small fields is challenging due to the interference in measurements from the diodes and covered some of the features of the widely used BEAMnrc and DOSRZnrc codes and their uses in modeling diodes. O’Shea explained how EGSnrc Monte Carlo code was used in simulating an extendable electron multileaf collimator, as a replacement of the currently used applicator for modulated conformal electron therapy technique. Also, developments in using a fast macro Monte Carlo radiation transport algorithm for proton beam dose calculation were presented by Jacqmin at this session.

The meeting was attended by a young contingent of physicist and engineers who enjoyed sharing scientific knowledge at the conference and laughs at the pub. Unexpectedly, the weather was fantastic during all week in Dublin, which added to the enjoyment of the conference and the city.

Report from Zahara Martín-Rodríguez, Supercomputing Center of Galicia (CESGA)

- **BCS Fortran Specialist Group Meeting**

  29 September 2011, British Computer Society (BCS), London

  Website: [www.fortran.bcs.org/2011/agenda11.php#present](http://www.fortran.bcs.org/2011/agenda11.php#present)

  As a follow-on from the two events last year, the CPG co-sponsored a meeting with the Fortran Specialist Group of the BCS. This was held on the afternoon of 29th September 2011 in the BCS’s London office near The Strand. Fuller details and copies of the presentations are available online (see below) but a brief summary is presented here.

  The talks opened with a light-hearted presentation by Jane Sleightholme who recounted tales of travelling - with her colleague Ian Chivers - to far flung (and usually cold) corners of the globe to train scientists and engineers in the dark arts of Fortran programming. Jane and Ian have very good insight into the use and uptake of Fortran in many international institutions and were able to provide descriptions of typical compilers and hardware that they encounter.

  John Reid gave two talks about developments in the Fortran standards from his perspective as ISO WG5 Convener no less. Both of these talks were in regards to Technical Reports (TRs) - or Technical Specifications under newly adopted terminology - these are effectively annexes to the standard and which may be fully encorporated at a later release. The first of these was in regards further interoperability with C - specifically to enable C functions to accept arguments of any rank or any type. He reported that he expects this TR to be approved next year as there does not appear to be any substantive objections. The standards process is a democratic one and requires consensus from the international representatives.

  John has been a key champion of coarrays - a means of adding explicit parallelism into Fortran code. These now exist in the Fortran 2008 standard. Many desirable features were omitted from the standard but these are now being addressed via a Technical Specification - "Enhanced Parallel Computing Facilities". This will now have been considered by the J3 committee, since the September meeting.

  David Muxworthy continued on the theme of standards work. He stated that the Programming Language Subcommittee of ISO has produced a report ‘Guidance to Avoiding Vulnerabilities in Programming Languages through Language Selection and Use’. This seeks to identify typical shortcomings and common errors in the use of specific programming languages and the Fortran WG5 committee is now updating and expanding their previous draft contribution.

  It is hoped that the next joint meeting between the CPG and the Fortran SG will take place in London on the 15th June 2012.

Report from John Pelan, Gatsby Computational Neuroscience Unit
Upcoming events of interest

• **Condensed Matter and Materials Physics (CMMP) conference 2011**

  13-15 December 2011, Lancashire County Cricket Club, Manchester, UK
  Website: [www.cmmp.org.uk](http://www.cmmp.org.uk)

  CMMPP11, with a wide range of symposia will reflect the breadth of condensed matter and materials physics this series of conferences attracts the highest quality invited and plenary talks, and offers a forum for student presentations.

  The conference will cover all areas related to condensed matter and materials physics, and their computational modelling.

• **Theory, Modelling and Computational Methods for Semiconductors (TM-CSIII)**

  18-20 January 2012, School of Electronic and Electrical Engineering, University of Leeds, UK
  Website: [www.tmcsuk.org/TMCSIII/TMCSIII.html](http://www.tmcsuk.org/TMCSIII/TMCSIII.html)

  A training day for PhD students and early career researchers will be held on day 1, followed by 2 days of contributed, poster and invited presentations. Topics will include:

  - Density Functional Theory Calculations
  - Tight Binding, Pseudopotential and Effective Mass Models for Electronic Structure
  - Empirical Potential Methods for Calculation of Structural Properties
  - Multiscale Approaches
  - Optical and Transport Properties of Quantum Nanostructures including Colloidal and Nanotubes
  - Dilute Magnetic Semiconductors
  - Graphene
  - Laser Devices
  - Photonic Structures
  - Plasmonics
  - Electronic Devices

• **Institute of Physics Plasma Physics Group conference 2012**

  2-5 April 2012, St Hugh’s College, University of Oxford, Oxford, UK
  Website: [plasma12.iop.org](http://plasma12.iop.org)

  The 2012 Annual plasma physics conference - covering magnetic and inertial fusion, high energy density physics, astrophysical and industrial plasmas.

  This popular event follows previous conferences in the series. The 38th IOP Annual Plasma Physics conference took place in North Berwick on April 2011 and was organised by the Atoms Beams and
Plasmas Group of the Department of Physics at the University of Strathclyde on behalf of the IoP Plasma Physics Group. The event provided an interesting and diverse programme for all scientists working in the field of plasma science, and is particularly intended to help progress and develop the careers of post doctoral and research students.

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• Monte Carlo Treatment Planning (MCTP) 2012

Third European Workshop on Monte Carlo Treatment Planning
15-18 May 2012, Seville, Spain
Website: www.mctp2012.com

The Third European Workshop on Monte Carlo Treatment Planning will be hosted by the city of Seville. We believe that a third meeting like the one we are going to celebrate next year, reinforces the original idea of establishing a working network for discussion and exchange of scientific knowledge focused on the application of Monte Carlo method to radiotherapy practice.

From the first meeting in Ghent, Belgium in 2006, and after the last one in Cardiff in 2009, the role of Monte Carlo in radiotherapy planning has continued growing and becomes more relevant every day, as new techniques are more sophisticated and ambitious. IGRT and 4-D planning are facing new cumulative uncertainties which require accurate calculations to justify the additional workload involved.

This Workshop on MCTP of the European Workgroup (EWG-MCTP) is addressed to offer the opportunity to scientists to exchange information, and to generate international collaborations. Our dual goal is to achieve the highest scientific level in the framework of a memorable stay in our city.

Workshop information, goals, abstract submission, preliminary programme are available from now on and will be updated on the website.

• Hermes 2012 Material Modeling Summer School

Website: http://hermes2012.org/

In 2012, London will play host to a unique four-day summer school for the world’s leading materials modelling Ph.D. students. This student-led event, held during the Olympic Games, focuses on two important issues: bringing together people and ideas from across different length scales; and communicating science to the general public. The participants will present their research, attend master classes given by internationally renowned academics, and develop their ability to communicate science. The invited speakers at the event will include Professor Craig Carter from MIT, who will be presenting multiscale modelling techniques for electrode materials used in next generation batteries, as well as Professor Chris Pickard from UCL, renowned for his pioneering contributions to the DFT package CASTEP.

Applications are now open, with a reduced rate if you register early. For more information about the event visit the website.
The consequences of magnetism on the mechanical properties of iron and its alloys are of major interest at present. Density functional theory can play a vital role in providing reliable reference data, but is inherently limited to system sizes up to a few hundred atoms. On the other hand, the important defects of iron alloys (such as dislocations, voids, loops, and inclusions) require many more atoms to be considered if they are to be treated accurately. Although empirical potentials can access the required length scale, it is very difficult to construct such potentials for systems in which the magnetism can vary. As a result, tight-binding models that explicitly include magnetism have received a great deal of attention. However, building and using magnetic tight binding models is not simple, and considerable effort is now taking place across Europe at present to find models and methods that work. In this meeting we will explore the state of the art of magnetic tight binding by bringing together the groups now active in this area. This is a joint IoP, Thomas Young Centre and ICAMS event.

Computational Physics Group Committee

Hans Fangohr  
Vera Hazelwood (Thesis prize)  
Andrew Horsfield  
Paul Hulse  
Geraint Lewis (Chair)  
Ian Morrison  
John Pelan  
David Quigley  
Jesus Rogel (Secretary)  
David Shipley (Newsletter)  
Nathan Sircombe (Treasurer)

We welcome expressions of interest for new committee members. If you are interested in joining the committee or require further information about the committee activities then please contact the Group Secretary Jesus Rogel.

IoP Computational Physics Group links

- Group webpages:  
  www.iop.org/activity/groups/subject/comp

- Newsletters:  
  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 the editor David Shipley (david.shipley@npl.co.uk)
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](www.aps.org/units/dcomp/newsletters/index.cfm)

- Europhysicsnews newsletter of the European Physical Society (EPS):
  [www.europhysicsnews.org/](www.europhysicsnews.org/)

- Newsletter of the Psi-k (Ψₖ) network:
  [www.psi-k.org/newsletters.shtml](www.psi-k.org/newsletters.shtml)

- The bulletin of the Knowledge Transfer Network for Industrial Mathematics, providing information for industrial and academic collaborators on recent results, milestones and opportunities. The full bulletin is available at:
  [www.industrialmath.net/content/news](www.industrialmath.net/content/news)

- 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/](www.thomasyoungcentre.org/events/)