Newsletter

Modelling of Block Copolymer Systems with Cell Dynamics

Newsletter Contents

Figure on cover:

Computer simulated nano-containers (background and four structures forming a square) by Marco Pinna and experimental images from the group of Prof. Alexander Boker, RWTH Aachen University, Germany. The nano-structures are formed by 'wrapping up' a block copolymer film around a nano-size spherical particle. Image design: Stephanie Hiltl, RWTH Aachen University, Germany. A more detailed description can be found in the lead article starting on page 1 in this edition of the newsletter.

This Newsletter . . .

Dear Newsletter Readership,

as usual, this newsletter and older newsletters can be found online at http://www.soton.ac.uk/~fangohr/iop_cpg.html, and most URLs mentioned in the newsletter are hyperlinks: clicking on them should take you to the corresponding webpage.

The *main feature* (page 1) of this newsletter is an invited contribution from Dr Marco Pinna who has won the 2009 PhD thesis prize as annually awarded by the Computational Physics Group.

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

The Computational Physics Group Committee.

Modelling of Block Copolymer Systems with Cell Dynamics

Abstract

In this review we illustrate a computer simulation method applied to a set of physical phenomena occurring in various block copolymer systems. The method is Cell Dynamics Simulation (CDS), which we implemented in a parallel computer program and further developed when necessary. The choice of CDS is due to the fact that it is a simplest minimal model of the Ginzburg-Landau type and its ability to describe complex physical situations was debated. We clarify this issue by a systematic study of diblock copolymers subjected to the external influences such as electric field, shear flow, confining surfaces and nanoparticles. Our results prove that CDS can describe such complex phenomena rather well and therefore, is a complementary method to other more elaborate techniques. This provides a ground for a future development of a tandem simulation where a very fast CDS method can be used as a precursor to more elaborate but slow techniques as, for instance, Dynamics Self-Consistent Field Theory.

Motivation of the study

Using soft materials is one of recent directions in nano-technology. Self-organisation in Soft Matter serves as a primary mechanism of structure formation. A new challenge is the preparation of nanosize structure for the miniaturisation of device and electronic components, [1,2,3] for production of masks for nanolithography, fabrication of nanoporous membranes for advanced separation media and photonic crystals. [1,2,4,5] We are interested in structures formed by polymers consisting of several chemically different blocks - block copolymers (see Fig.1). Block polymers are chain molecules which are composed of chemically different blocks covalently connected to one macromolecule. They belong to an important class of materials, that due to their natural ability of microphase separation can self-assembly into different structures on the scale of their blocks which is in the range of 10-100 nm. [1] These can be very simple structures as lamellae, spheres, packed cylinders, and more complex structures such as gyroid, etc (see Fig.2). Block copolymer systems have been studied for several decades in a vast number of experimental and theoretical works. [6,7,8,9,10,11,12] The research is driven by the desire to tailor a certain morphology. The control of long-range order in structures is very important for practical applications in chemistry, materials science and for bio-mimicking applications. For instance, the use of block copolymers in electronic and photonic applications requires production of highly ordered and defect-free structures. [3] External fields are promising candidates to achieve that goal. Such fields can be surface fields, [1, 13, 14] electric field [1, 13, 15, 16, 17, 18, 19] and shear flow. [13, 15, 16, 20, 21, 22] Prediction of the structure formation in copolymer melts is one of the goals of soft condensed matter physics. These experiments are very difficult and computer modelling guidance can help to understand structure formation in
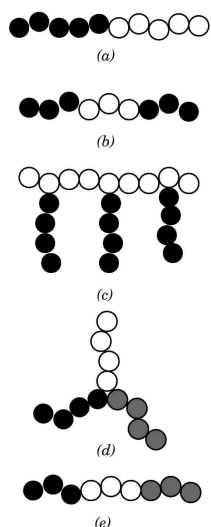
Figure 1: Schematic representation of several block copolymer architectures. The white and black beads represent monomer A or B respectively. (a) AB diblock copolymer, (b) ABA triblock copolymer, (c) grafted (branched) AB copolymer, (d) star ABC triblock copolymer and (e) linear ABC triblock copolymer.

the block copolymers. We aim to understand structure formation in block copolymers
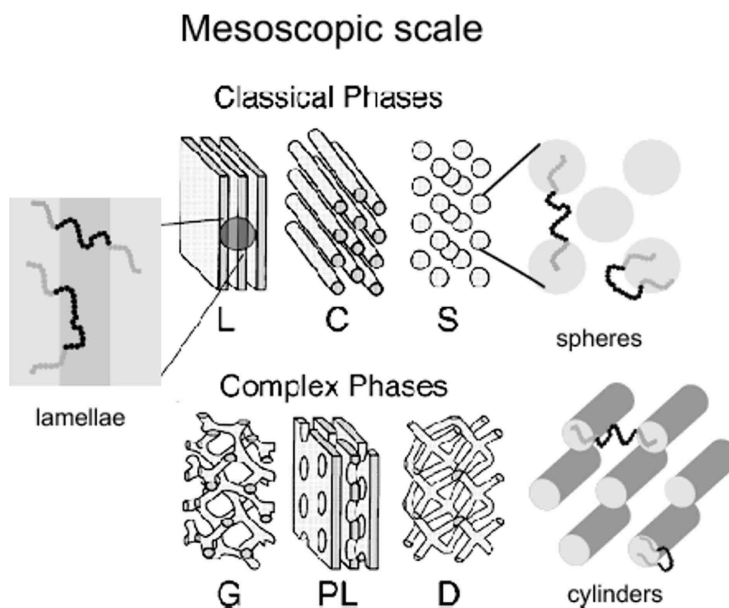
Figure 2: Block copolymers structures on a mesoscopic scale. The structures are: lamellae (L), cylinders (C), spheres (S), gyroid (G), perforated lamellae (PL) and double diamond (D).

systems by means of computer simulation. In spite of many simulation techniques developed until now the field offers a vast quantity of open questions, some of which we address in the present thesis. We want to create a fast parallel code, which would serve as a 'precursor' for other heavier simulation methods.

The Cell Dynamics Simulation

In the last decades, many different computer modelling methods have been developed. Some are very accurate but very slow, others are very fast and less accurate but not less useful. [1] Latter ones are mesoscopic simulation methods which can describe the behaviour of block copolymers on a large scale. One of these methods is the Cell Dynamics Simulation (CDS). The cell dynamics simulation is widely used to describe the mesoscopic structure formation of diblock copolymer systems. [23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33] The Cell Dynamics Simulation is reasonably fast and can be performed in relatively large boxes. However, experimental size systems and experimental times cannot be achieved even with this method on modern single processor computers. To link simulation results to experiments it is necessary to use very large simulation boxes. The only way to achieve this goal is to create a computer program, which can run on many processor in parallel.

In the cell dynamics simulation an order parameter $\psi(t, i)$ is determined at time t in cell i of a discrete lattice. For AB diblock copolymer we use the difference between local and global volume fractions:

$$\psi = \phi_A - \phi_B + (1 - 2f) \tag{1}$$

where ϕ_A and ϕ_B are the local volume fraction of A and B monomers respectively, and f is the volume fraction of A monomers in the diblock, $f = N_A/(N_A + N_B)$.

The time evolution of the order parameter is given by a Cahn-Hilliard-Cook (CHC) equation: [25, 26]

$$\frac{\partial \psi}{\partial t} = M\nabla^2 \left(\frac{\delta F[\psi]}{\delta \psi} \right) + \eta \xi(\mathbf{r}, t) \tag{2}$$

where M is a phenomenological mobility constant. Here we set M=1 which correspondingly sets the timescale for the diffusive processes (the dimensionless time is tM/a_0^2, where the lattice cell size a_0 is set to 1). The last term in Eq. 2 is a noise term where η is the amplitude of the noise and $\xi(\mathbf{r}, t)$ is a normalised Gaussian random noise, which satisfies the fluctuation-dissipation theorem. In Eq. 2 $F[\psi]$ is the free energy functional divided by kT, which can be written as: [24]

$$
\begin{aligned}
F[\psi(\mathbf{r})] &= \int d\mathbf{r}[H(\psi) + \frac{D}{2}|\nabla\psi|^2] \\
&+ \frac{B}{2} \int d\mathbf{r} \int d\mathbf{r}' G(\mathbf{r} - \mathbf{r}')\psi(\mathbf{r})\psi(\mathbf{r}')
\end{aligned}
\tag{3}
$$

where the coefficient D is a positive constant, the Green function $G(\mathbf{r} - \mathbf{r}')$ for the Laplace equation satisfies $\nabla^2 G(\mathbf{r} - \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}')$, B is a parameter that introduces a
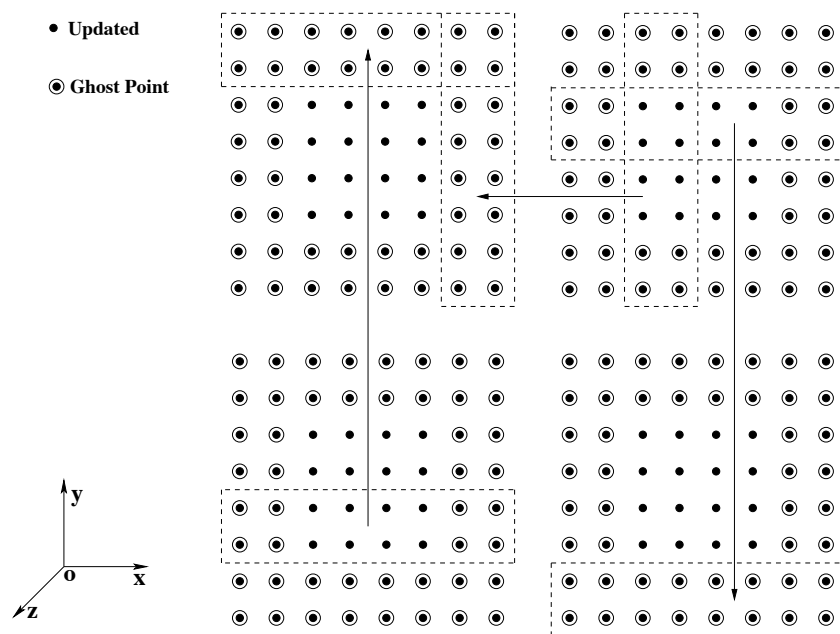
Figure 3: The domain decomposition of 8^3 grid as viewed in x-y plane. The grid is subdivided into 8 subgrids (only 4 are seen in the x-y plane). The ghost points are added to each of subgrids. The communications between processors in x-y plane are indicated by the arrows. Copyright 2007, Wiley-VCH Verlag GmbH & Co. KGaA. Reproduced with permission.
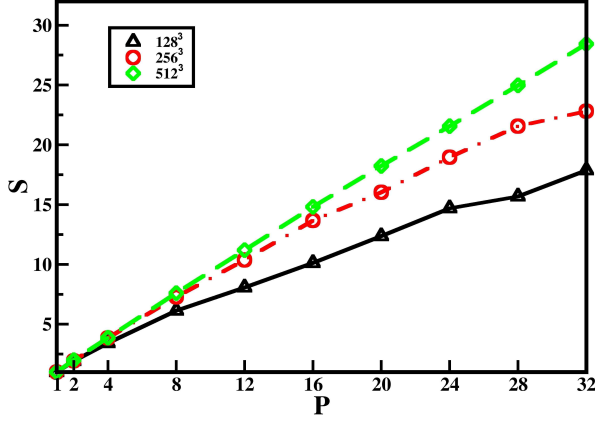
Figure 4: The speedup $S = S(m, P)$ versus number of processors P for three different grid sizes in 2D with single copy optimization. Copyright 2007, Wiley-VCH Verlag GmbH & Co. KGaA. Reproduced with permission.

chain-length dependence to the free-energy, [27] and $H(\psi)$ is the free energy: [27]

$$H(\psi) = [-\frac{\tau}{2} + \frac{A}{2}(1 - 2f)^2]\psi^2 + \frac{v}{3}(1 - 2f)\psi^3 + \frac{u}{4}\psi^4 \tag{4}$$

Here τ is a temperature parameter and A, v, u are phenomenological constants. [28] All these parameters can be related to molecular characteristics. [34]

If we add a steady shear defined by:

$$\mathrm{v_z} = \dot{\gamma}y, \ \mathrm{v}_x = \mathrm{v_y} = 0 \tag{5}$$

where we take the z-axis in the flow direction, y-axis in the velocity gradient direction. Thus the x-axis is the vorticity axis.

When an electric field along the x-axis is applied and no flow is present, the evolution equation similar to Eq. 2 for diblock copolymer melt becomes: [35,36]

$$\frac{\partial \psi}{\partial t} = \tilde{\alpha}\nabla_x^2(\psi) + \nabla^2\left(\frac{\delta F(\psi)}{\delta \psi}\right) + \eta\xi(\mathbf{r}, t) \tag{6}$$

where

$$\tilde{\alpha} = \frac{\varepsilon_0 v_0 E_0^2}{kT}\frac{(\varepsilon_A - \varepsilon_B)^2}{\varepsilon_A f + \varepsilon_B(1 - f)} \tag{7}$$

Here ε_0 is the vacuum permittivity, v_0 is the volume of one polymer chain, ε_A and ε_B are the dielectric constants of the blocks A and B respectively, and E_0 is the strength of the electric field.

It is difficult to implement a real time and experimental-scale simulation with traditional serial algorithms because of the expensive computation. In our work a parallel, spatial decomposition based algorithm for large scale CDS is proposed. [37,38] With the efficient strategy of domain decomposition (see Fig.3) and the fast method of neighbouring points location we greatly reduce the calculating and communicating cost (see Fig.4). The numerical results indicate that the proposed parallel algorithm
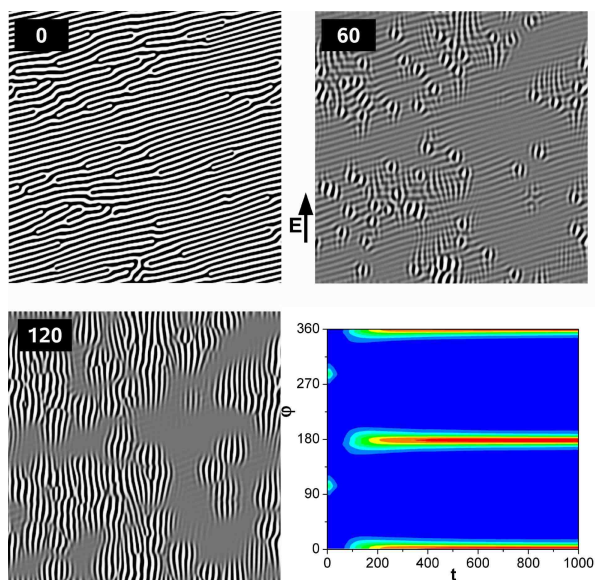
Figure 5: Example of one of the mechanisms of lamellae reorientation under electric field: Nucleation and growth with partial melting. It confirms, that defects serve as nucleation sites. The direction of the electric field is indicated by the arrow. The electric field was switched on at $t = 0$ (elapsed time t is shown in black rectangles). Time development of the scattering intensity as a function of the azimuthal angle φ in the presence of the electric field is shown in the right bottom image. Copyright 2009, The Royal Society of Chemistry. Reproduced with permission.

can provide an efficient way for computer simulation of block copolymers systems of experimental size.

Applications

We investigate several physical phenomena with the CDS code.

We demonstrate that two mechanisms of lamellae reorientation observed experimentally under applied electric field [39] which have been previously described within Dynamic Self Consistent Field Theory [36] can be fully explained with a much more simple model with the Ginzburg-Landau Hamiltonian. A third alignment mechanism has been identified which was not previously reported. [40] A more complete picture of reorientation under electric field emerges that clarifies the crucial role of structural defects (see Fig.5).

In our work the Cell Dynamics Simulation is used to investigate pathways of Sphere-to-Cylinder transition in block copolymer melt under applied simple shear flow and electric field. [15] Both fields can induce the transition when their strength is above some critical value. At weak fields the spherical phase is to be preserved, with spheres being deformed into ellipsoids. Weak shear flow is found to improve order in spherical phase. Observed sliding of layers of spheres under shear (see Fig.6) is very similar to the experimental finding by Hamley et al. [2] The kinetic pathways are sensitive to the degree of microphase separation in the system and hence affected by tempera-

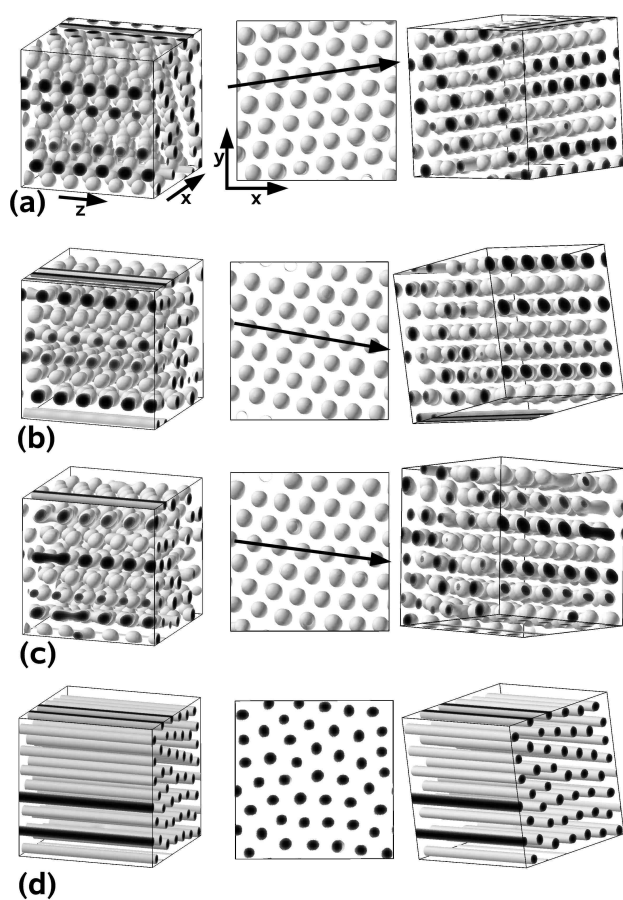Figure 6: Diblock copolymer sphere phase under shear flow for different shear along the z-axis (increasing from (a) to (d)). The middle column shows the vorticity plane view. The arrows inside the pictures indicate the view direction for the Fig.6,right, which shows different orientation of simulated box for a better observation of sliding sphere layers. Copyright 2006, American Institute of Physics. Reproduced with permission.
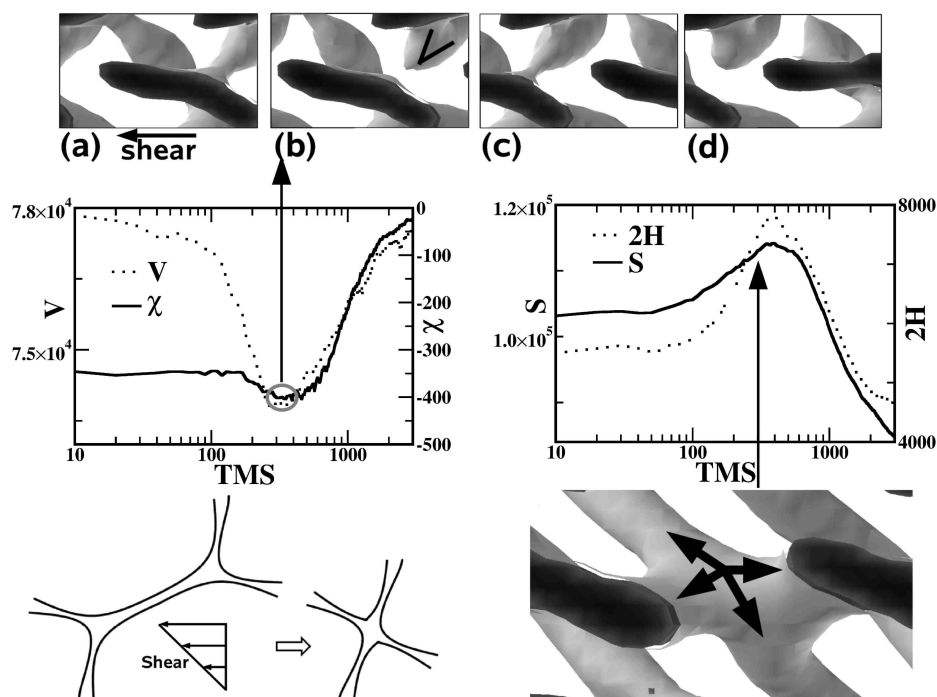
Figure 7: Example of gyroid transformation under shear and its quantitative analysis with Minkowski functionals. Top: Crops of the simulation boxes. 'V' indicates a V-shape connection. Images illustrate the reconnection propagation as time increases from (a) to (d). Middle: Minkowski Functionals as function of time steps. Bottom: cartoon and snapshot illustrate formation mechanism of four-bond connection. Copyright 2008, The Royal Society of Chemistry. Reproduced with permission.

ture. The details of the pathways can be described in detail by means of Minkowski functionals. [15]

We use the Cell Dynamics Simulation we investigate cubic gyroid morphology (perhaps, the most fascinating one amongst simple morphologies) in block-copolymer melts under simple shear flow and electric field. The electric field should be stronger than a certain critical value to induce transition to a cylindrical phase. In the case of simple steady shear the Gyroid-to-Cylinder transition was observed even for a very weak shear. Quantitative analysis of pathways of Gyroid-to-Cylinder transition is performed by means of Minkowski functionals (see Fig.7). We found that the kinetics of the Gyroid-to-Cylinder transition is different under electric field and shear flow. Moreover, the gyroid structure under different strengths of electric field shows different pathways. Different types of intermediates as five-, four-fold (see Fig.7) connections and 'winding' cylinders are found for different pathways. [16]

Using Cell Dynamics computer simulation we perform a systematic study of thin
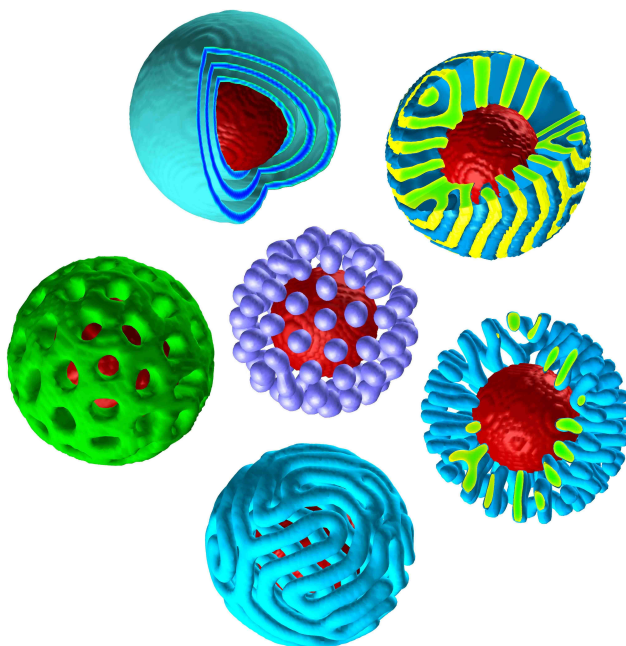
Figure 8: Examples of nano-containers.

block copolymer films around a nanoparticle. Lamellar-, cylinder-, and sphere-forming block copolymers are investigated for different film thicknesses, particle radii and boundary conditions at the film interfaces. The obtained structures include: standing lamellae and cylinders, 'onions', cylinder 'knitting balls', 'golf-ball', layered spherical, [41] 'virus'-like and mixed morphologies with T-junctions and U-type defects. Kinetics of the structure formation and difference with planar thin films are discussed. Our simulations suggest that novel porous nano-containers can be formed by the coating of a sacrificial nano-bead by a block copolymer layer with a well controlled nanostructure (see Fig.8). Recently these findings were confirmed by experiments. [42] These containers can serve as nano-reactors in catalysis or nano-envelopes for drug delivery.

Another confinement geometry, which attracts extensive attention in recent years is cylindrical nano-pores. We show that a simple Ginzburg-Landau type theory can predict a tremendous rich zoo of diblock copolymer morphologies in cylindrical nanopores (see Fig.9). Using the Cell Dynamics Simulation we study in detail lamellar-, cylinder- and eventually sphere-forming diblock copolymers melts in cylindrical nanopores. [43] This very fast simulation method is proposed to be used as a research precursor for more elaborate computational techniques.

In the last example of complex block copolymer systems studied with CDS we show that the interaction between diblock copolymer and nanoscopic particles can lead to the formation of hybrid materials. The morphology of such hybrid materials depends on the polymer compositions as well as on shapes, sizes, and surface treat-
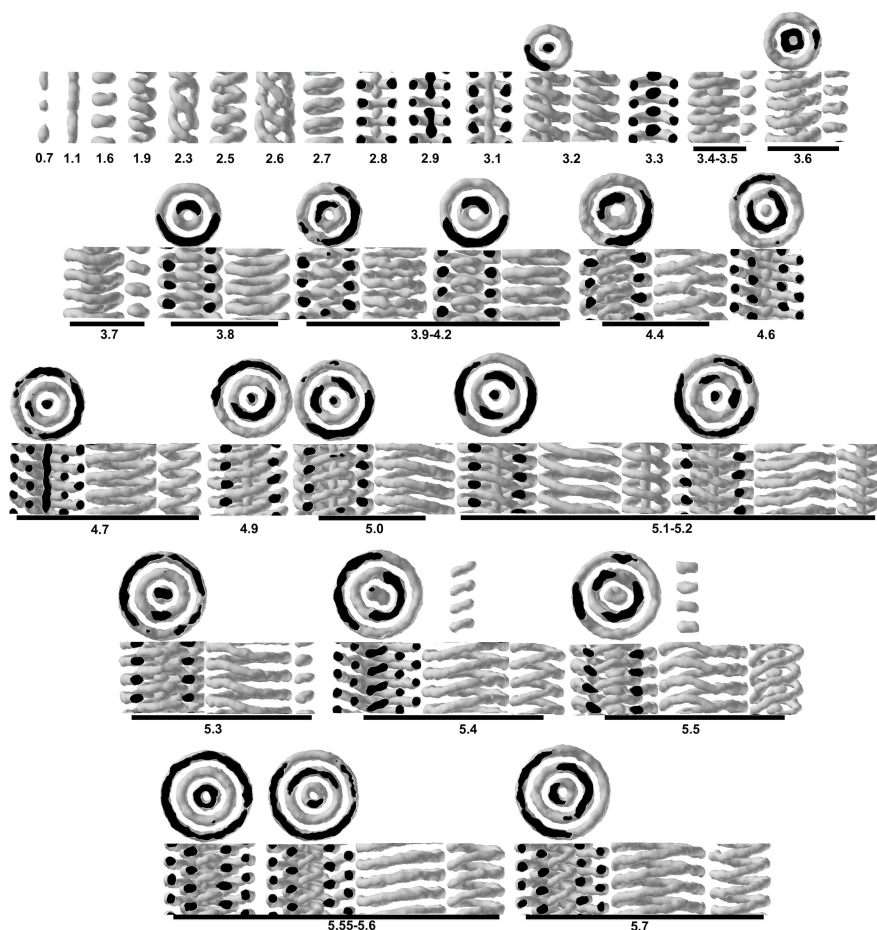
Figure 9: Examples of structures formed by cylinder morphology of block copolymers in cylindrical nano-pores. Numbers are ratio of the pore diameter to the domain spacing. For complex multilayer structures some of the internal layers are shown to the right of the main image with the top view shown above the main image. Copyright 2009, American Institute of Physics. Reproduced with permission.
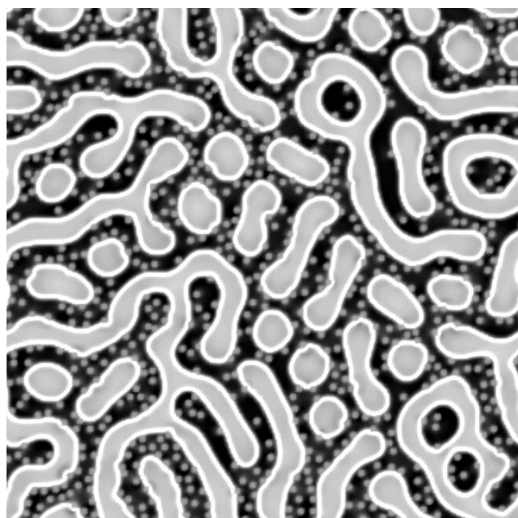
Figure 10: Example of nano-particle/diblock copolymer hybrid material.

ment of the particles (see Fig.10). We propose a hybrid mesoscopic approach to study the dynamics of nanocomposites composed from a block copolymer melt and a suspension of nanocolloids. We combine a collective description of the polymer dynamics with the individual resolution of the nanocolloids. We implemented the method in two dimensions and tested it for different particle sizes, diblock copolymer composition and polymer-colloid interaction. [44]

Conclusions

It was believed that relatively simple Landau-Ginzburg type simulation approaches are too crude to accurately describe complex dynamical behaviour observed in block copolymer nanostructures. However, that belief nether was ever verified, nor the limits of such approaches were determined. We implemented such a simulation approach (Cell Dynamics Simulation) as a highly scalable parallel code, and extended it to describe confined systems and systems under external fields. We found that CDS is well capable of accurate describing of often very complex dynamical behaviour in a large set of chosen systems. Therefore, CDS should not be opposed by a more elaborate simulation approaches, such as for instance Dynamic Self-Consistent Field Theory, but rather be used in addition to them to form a simulation tandem. That would allow to enormously speed up research time for the systems with multi-dimensional parameter space.

The work described here is a summary of what was developed during my PhD study, and further details can be found either in the original papers [15, 16, 37, 38, 40, 41, 42, 43] or in a separately published book. [44]

References

[1] *Nanostructured Soft Matter*; Zvelindovsky, A. V., Ed.; Springer, Dordrecht, 2007.

[2] Hamley, I. W.; Pople, J. A.; Fairclough, J. P. A.; Terrill, N. J.; Ryan, A. J.; Booth, C.; Yu, G.-E.; Diat, O.; Almdal, K.; Mortensen, K.; Vigild, M. *J. Chem. Phys.* **1998**, *108*, 6929.

[3] Segalman, R. A. *Material Science and Enginering R* **2005**, *48*, 191.

[4] Park, C.; Yoon, J.; Thomas, E. L. *Polymer* **2003**, *44*, 6725.

[5] Urbas, A.; Sharp, R.; Fink, Y.; Thomas, E. L.; Xenidou, M.; Fetters, L. J. *Advanced Materials* **2000**, *12*, 812.

[6] Qi, S.; Wang, Z. W. *Phys. Rev. E* **1997**, *55*, 1682.

[7] Matsen, M. W. *J. Chem. Phys.* **2001**, *114*, 8165.

[8] M. Nonomura, K. Y.; Ohta, T. *J. Phys.:Condens. Matter* **2003**, *15*, L423.

[9] Yamada, K.; Nonomura, M.; Ohta, T. *Macromolecules* **2004**, *37*, 5762.

[10] Yamada, K.; Nonomura, M.; Saeki, A.; Ohta, T. *J. Phys.: Condens. Matter* **2005**, *17*, 4877.

[11] Schick, M. *Physica A* **1998**, *251*, 1.

[12] Vigild, M. E.; Almdal, K.; Mortsen, K.; I. W. Hamley, J. P. A. F.; Ryan, J. *Macromolecules* **1998**, *31*, 5702.

[13] Sakurai, S. *Polymer* **2008**, *49*, 2781.

[14] Fasolka, M. J.; Mayes, A. M. *Ann. Rev. Mat. Res.* **2001**, *31*, 323.

[15] Pinna, M.; Zvelindovsky, A. V.; Todd, S.; Goldbeck-Wood, G. *J. Chem. Phys.* **2006**, *125*, 154905.

[16] Pinna, M.; Zvelindovsky, A. V. *Soft Matter* **2008**, *4*, 316.

[17] Matsen, M. W. *Soft Matter* **2006**, *2*, 1048.

[18] Schmidt, K.; Böker, A.; Zettl, H.; Schubert, F.; Hansel, H.; Fischer, F.; Weiss, T. M.; Abetz, V.; Zvelindovsky, A. V.; Sevink, G. J. A.; Krausch, G. *Langmuir* **2005**, *21*, 11974.

REFERENCES

[19] Böker, A.; Elbs, H.; Hansel, H.; Knoll, A.; Ludwigs, S.; Zettl, H.; Zvelindovsky, A. V.; Sevink, G. J. A.; Urban, V.; Abetz, V.; Muller, A. H. E.; Krausch, G. *Macromolecules* **2003**, *36*, 8078.

[20] Zvelindovsky, A. V.; Sevink, G. J. A.; van Vlimmeren, B. A. C.; Maurits, N. M.; Fraaije, J. G. E. M. *Phys. Rev. E* **1998**, *57*, R4879.

[21] Morozov, A. N.; Zvelindovsky, A. V.; Fraaije, J. G. E. M. *Phys. Rev. E* **2000**, *61*, 4125.

[22] Zvelindovsky, A. V. M.; Sevink, G. J. A. *Europhys. Lett.* **2003**, *62*, 370–376.

[23] Oono, Y.; Puri, S. *Phys. Rev. A* **1988**, *38*, 434.

[24] Bahiana, M.; Oono, Y. *Phys. Rev. A* **1990**, *41*, 6763.

[25] Ohta, T.; Enomoto, Y.; Harden, J. L.; Doi, M. *Macromolecules* **1993**, *26*, 4928.

[26] Kodama, H.; Doi, M. *Macromolecules* **1996**, *29*, 2652.

[27] Hamley, I. W. *Macromol. Theory Simul.* **2000**, *9*, 363.

[28] Ren, S. R.; Hamley, I. W. *Macromolecules* **2001**, *34*, 116.

[29] Ren, S. R.; Hamley, I. W.; Teixeira, P. I. C.; Olmsted, P. D. *Phys. Rev. E* **2001**, *63*, 041503.

[30] Ren, S. R.; Hamley, I. W.; Sevink, G. J. A.; Zvelindovsky, A. V.; Fraaije, J. G. E. M. *Macromol. Theory Simul.* **2002**, *11*, 123.

[31] Feng, J.; Liu, H.; Hu, Y. *Macromol. Theory Simul.* **2002**, *11*, 549.

[32] Feng, J.; Liu, H.; Hu, Y. *Macromol. Theory Simul.* **2002**, *11*, 556.

[33] Feng, J.; Ruckenstein, E. *J. Chem. Phys.* **2004**, *121*, 1609.

[34] Ohta, T.; Kawasaki, K. *Macromolecules* **1986**, *19*, 2621.

[35] Lyakhova, K. S.; Zvelindovsky, A. V.; Sevink, G. J. A. *Macromolecules* **2006**, *39*, 3024.

[36] Zvelindovsky, A. V.; Sevink, G. J. A. *Phys. Rev. Lett.* **2003**, *90*, 049601.

[37] Guo, X.; Pinna, M.; Zvelindovsky, A. V. *Macromol. Theory Simul.* **2007**, *16*, 779.

[38] Guo, X.; Pinna, M.; Zvelindovsky, A. V. In: *Parallel Scientific Computing and Optimization: Advances and Applications. Springer Series in Optimization and Its Applications*; Springer: New York, 2009; Vol. 27, pp 253–262.

REFERENCES

[39] Böker, A.; Elbs, H.; Hansel, H.; Knoll, A.; Ludwigs, S.; Zettl, H.; Urban, V.; Abetz, V.; Muller, A. H. E.; Krausch, G. *Phys. Rev. Lett.* **2002**, *89*, 135502.

[40] Pinna, M.; Schreier, L.; Zvelindovsky, A. V. *Soft Matter* **2009**, *5*, 970.

[41] Pinna, M.; Guo, X.; Zvelindovsky, A. V. *Polymer* **2008**, *49*, 2797.

[42] Pinna, M.; Hiltl, S.; Guo, X.; Boker, A.; Zvelindovsky, A. V. *ACS Nano* **2010**, *4*, 2845.

[43] Pinna, M.; Guo, X.; Zvelindovsky, A. V. *J. Chem. Phys.* **2009**, *131*, 214902.

[44] Pinna, M. *Mesoscale modelling of block copolymer systems*; VDM Verlag Dr Muller, Saarbrucken, 2010.

Computational Physics Group News

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.

The annual deadline for applications is 1 March.

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

The Computational Physics Thesis Prize 2010

The Committee of the Institute of Physics Computational Group offers 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 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 2010.
- ▷ The submission deadline is April 30th 2011.

Submission format

- ▷ 4 page (A4) abstract
- ▷ citation from PhD supervisor (up to 1 A4 page)
- ▷ confidential report from external thesis examiner (up to 1 A4 page).

Please enclose contact details, including an email address. Further details may be requested from shortlisted candidates.

Submission Address

> ▷ Dr Vera Hazelwood
>
> KTN for Industrial Mathematics
>
> Vera.hazelwood@industrialmaths.net

The Computational Physics Thesis Prize 2009
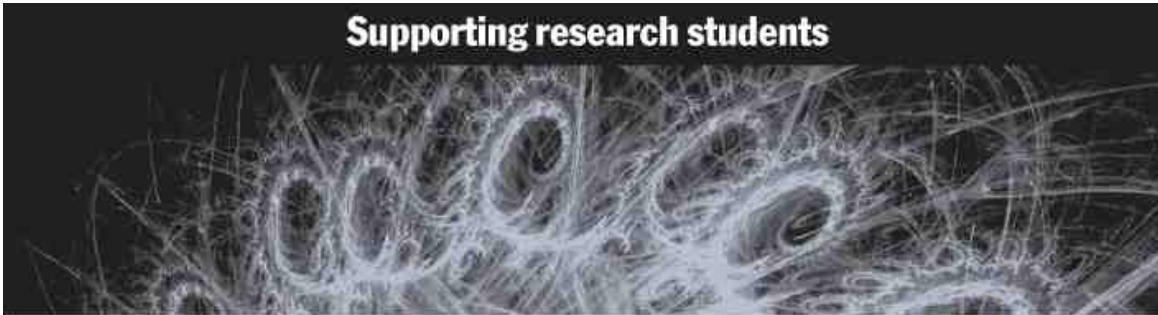
The Winner of the Computational Physics Thesis Prize 2009 is Dr Marco Pinna with his work on Modelling of Block Copolymer Systems with Cell Dynamics, a part of which is described in the lead article of this edition (page 1). Marco earned a doctorate from the University of Central Lancashire where he continues as a research associate in computational physics. Congratulations!

IoP Computational Physics Group - Research Student Conference Fund (Travel awards)

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/about/grants/research_student/page_38808.html`

Conference and workshop reports

CECAM Workshop on Approximate Quantum Methods

▷ 20 - 24 September 2010, Bremen, Germany

A workshop on Approximate Quantum Methods was held in Bremen from September 20th to 24th, 2010. The meeting was organised by Prof. Thomas Frauenheim of the Bremen Center for Computational Materials Science, and successfully brought together leading figures working on the development of approximate semiempirical and DFT-based methods, and hybrid quantum mechanics / molecular mechanics approaches. The workshop was attended by about 80 researchers and students from across the world. The programme comprised more than 30 invited oral presentations, distributed over four days, and about 25 posters, which were presented at an evening poster session. Topics of discussion focussed on recent advances and insights into existing approximate quantum methods, as well as efforts to develop new approaches, and the successes of current and new methodologies in understanding chemical reaction mechanisms, modelling excited states, and describing photoexcitation and carrier dynamics. Also, much emphasis was placed on identifying critical challenges in the field, as well as future directions for research and development of next-generation computational tools. The strength of the programme meant that the meeting was very well attended, with the lecture halls being used to full capacity throughout the week. A friendly and harmonious atmosphere was maintained throughout the workshop, which stimulated the sharing of scientific knowledge and the birth of new collaborations. The meeting was organised in a way that promoted such exchanges among its participants, almost from breakfast to dinner. Students and senior researchers alike thoroughly enjoyed the workshop; many commented highly about the venue, organisation, and scientific content.

Rafael Miranda, PhD student, University College London

Theory, Modelling and Computational methods for Semiconductors II (Jan 2010)

▷ 13-15 January 2010, York, UK

The second "Theory, Modelling and Computational methods for Semiconductors" workshop (TMCS II) was a great success with 50 delegates over the 3 days.

Most delegates were UK based but we also had an invited speaker from Finland (Risto Nieminen), another one from Ireland (Eoin OReilly), and contributed talks from Rome, Vienna, Ireland (4) and Spain.

A number of the international speakers originally scheduled to attend and present were in the end deterred by the threat of heavy snow in Yorkshire and cancelled their attendance in the 3 days prior to the workshop. Otherwise we would have welcomed almost 60 delegates in total.

The event was sponsored by the UK Car-Parrinello Consortium, the IoP Semiconductor Physics Group and the IoP Computational Physics group. Industrial sponsorship was provided by Accelrys Ltd Cambridge and Quantum Wise Copenhagen, both of whom had an exhibition and presentation of their software packages.

The event was held in St. Williams College, in the centre of York, next to the beautiful York Minster.

The first day of the workshop was dedicated to student training with 4 presentations 90 minutes long on topics in modelling of semiconductors at a PhD student level. These covered the range of topics that were going to be discussed in the next two days.

These talks were well received and around 25 attendees participated, most of which stayed for the regular workshop as well.

On the second and third days, we had a succession of talks (invited talks were 30 minutes long, contributed talks were 15 minutes) covering the range of current theoretical / computational research in semiconductors, including high-level GW theory of quantum transport, applications of DFT to study defects, semi-empirical methods to study quantum dots, photonic methods to study quantum cascade lasers, etc. There were also poster sessions, hands-on practical sessions with codes from Accelrys and QuantumWise, and a conference dinner.

Full details of the programme (including copies of the talks) are available at the TMCS website: http://www.tmcsuk.org/TMCS/TMCSII/TMCSII.htm.

In the closing discussions, it was decided that a TMCS-III conference should be organized in 2012 at the same time of year and with a similar format. An international advisory committee will be formed later this year to prepare the next conference.

Matt Probert

16th UK Monte Carlo User Group Meeting (MCNEG 2010)

▷ 12-13 April 2010, NPL, Teddington, UK

▷ Organised by: Mark Bailey and David Shipley

The 16th UK Monte Carlo User Group Meeting (MCNEG 2010) was held on 12-13 April 2010 at the National Physical Laboratory, Teddington, Middlesex, UK. The meeting continues a tradition of actually having something of an international flavour, with several of the 40 delegates attending from overseas including the two invited speakers, Katia Parodi (Heidelberg Ion Beam Therapy Centre, Heidelberg, Germany) who gave two talks, Recent and future developments of the FLUKA MC code for ion beam therapy and The role of Monte Carlo at the Heidelberg Ion Beam Therapy Center; and Professor Hooshang Nikjoo (Karolinska Institute, Stockholm, Sweden) who gave a presentation on Radiation track structure, DNA damage, and risk of exposure to ionizing radiations.

Presentations in this meeting were given over four themed sessions, covering Protons and Light Ions; Biological, Protection and Environmental; Radiotherapy and Imaging; and Small Fields and Microdosimetry. It was notable that the FLUKA code was used for several of the presentations and seems to be being used significantly more widely in many applications from radiotherapy to shielding, particle physics to criticality; it has a worldwide community now of over 2000 users. Delegates also had the opportunity to see the new clinical linac facility at NPL as well as some of the primary standards for ionising radiation currently in use. A enjoyable meeting dinner was held at Bar Estilo in Teddington, just a few minutes' walk from NPL, at the end of the first day.

Prizes (kindly provided by the Institute of Physics Computational Physics Group) were offered for the best presentations by students, and we are happy to report that Julien Smeets (ULB, Belgium) won first prize, with his presentation A PHITS-based dose calculation engine to evaluate the effect of inhomogeneities in prostate brachytherapy. Second and third prizes went to Thiansin Liamsuwan (Karolinska Institute, Sweden) and Leena Al-Sulaiti (NPL and the University of Surrey, United Kingdom) respectively.

The organisers are very grateful to the Institute of Physics (Computational Physics Group) and to Elekta plc, who supported the meeting.

David Shipley

Meetings organised jointly with the BCS Fortran Specialist Group

This year two events were jointly organised between the Computational Physics Group and the Fortran Specialist Group (FSG). Fortran remains a very important programming language in computational physics and numerics and the FSG is key promoter of Fortran as well as acting as a focal point for the standardisation effort in the UK.

Fortran in Physics - Its Legacy and its Future?

The first of these events was a full-day meeting held on Monday 7th June at the BCS offices in London. It was attended by circa forty people and even featured some live blogging by an audience member. As well as being the first of our joint meetings it also marked the 40th anniversary of the Fortran Specialist Group itself.

The first talk of the morning session examined the development and standardisation of Fortran over the last 40 years to-date. David Muxworthy, who is the Fortran convener of the British Standards Institute (BSI), described the changes from decade to decade and the challenging trials and tribulations of standardising a language from both a technical and social perspective. The most significant addition to the latest standard - namely co-arrays - was then dealt with by John Reid. John has had a long-standing role in the ISO

Fortran standards work and has championed co-arrays which adds explicit parallelism to Fortran using a well understood SIMD model (I believe that this is the first ISO standard language with explicit support for parallelism). It comes at a time where parallelism is now the only route to improved through-put now that the performance of single CPU cores has essentially reached a plateau.

Of course, Fortran as a standardised programming language would mean nothing if there weren't compilers for it. In the afternoon, Stephen Blair-Chappell from Intel's Compiler Labs discussed tools and techniques for getting increased performance from your code, largely using implicit parallelism and Intel's tool-chain to access multicore computing and various CPU performance features.

The focus for the afternoon was on applications in the physics domain, and the presentations were lead by Craig Lucas of the Numerical Algorithms Group Ltd. The NAG libraries are well known to Fortran programmers of course, but NAG also provide the Computational Science and Engineering (CSE) support team for HECToR, a national high-performance computing service run on behalf of the research councils. Their role is to help computational scientists get the most performance from their codes on the HECToR platform. Craig highlighted a wide range of physics related codes that were running on the service from a variety of fields including atomic, molecular and plasma physics.

At the end of the meeting there was an open discussion on the future of Fortran in the physics community. While there was no clear outcome, it was evident there

was a disconnect between the important role that Fortran continues to play in state-of-the-art computational physics and the lack of teaching and promotion of Fortran at undergraduate level. It was certainly perceived by some that science is suffering as a result of inadequate teaching of Fortran and computer programming skills in general at the earliest opportunity.

Full details of the meeting, including slides/presentations can be found here; http://www.fortran.bcs.org/2010/fortraninphysics.php

John Pelan

A Fortran Afternoon: Developing Code for Physics plus C Interoperability

The second joint event was held on Thursday, 30th September also at the BCS London offices. It was an afternoon of three talks which followed on from the FSG's AGM that morning.

The first talk was entitled "The CASTEP project: reflections on the first ten years" and was given by Keith Refson of the Rutherford Appleton Laboratory. CASTEP is a highly successful materials modelling code which uses density functional theory (DFT). As a fairly recent code, it is an excellent example of what can be achieved using modern Fortran and robust design and coding practices. Keith summarised the development methods and lessons learned to-date, both positive and negative, and without doubt, I think that anyone developing computational physics codes should review the experiences of the CASTEP team.

Jane Sleightholme presented an update to the regular compiler report that she produces with Ian Chivers. This work gives an overview of all the current Fortran compilers - free and commercial - and compares their feature-sets and conformance against the published standards (as stated by the compiler developers themselves). As such this work is useful for compiler selection and for tracing their development year-on-year.

Finally, the Fortran stalwart John Reid (of JKR Associates and Rutherford Appleton Laboratory) described the on-going work by the standards folk towards interoperability between Fortran and C at the API level. This work is in the form of a Technical Report - essentially a supplement to the current standard - and describes how data can be passed reliably between Fortran and C programs and how C library routines can be called from Fortran in a portable manner. John also described some other aspects of the standards work.

Full details of the meeting, including slides/presentations can be found at http://www.fortran.bcs.org/2010/agenda10.php#present.

John Pelan

Fortran 2008

The most recent Fortran standard (ISO/IEC 1539-1:2010), informally known as "Fortran 2008", was approved in September. Congratulations to all involved. New features include:

  ▷ Co-array Fortran - a parallel execution model (as described above).

  ▷ Submodules - new structuring features for modules

  ▷ `DO CONCURRENT` - enables declaration of non-interdependent iterations

  ftp://ftp.nag.co.uk/sc22wg5/N1801-N1850/N1830.pdf

55th Magnetism and Magnetic Materials 2010

  ▷ 13-18 November 2010

  ▷ Atlanta, GA, US
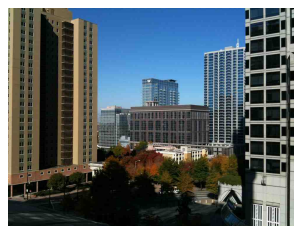
The 55th conference on Magnetism and Magnetic Materials (MMM2010) took place in Atlanta (US) in November 2010 with an approximate attendance of 600 researchers.

Topics that received wide interested included magnetoelectronic based on magnetic and spintronic logic elements and associated more fundamental research questions such as domain wall propagation in nanowires, spin-polarised currents, pure spin currents, perpendicular anisotropy and the role of finite temperatures. All research is heavily underpinned by computational models to explain observations at the nanoscale.

Russel Cowburn (Imperial College) gave a fascinating talk demonstrating a model for a new three-dimensional design of magnetic random access memory which has the potential to replace today's DRAM and provide a number of significant advantages. At this early stage of the device development all of the results that Russel presented in a very well attended invited talk were based on computer simulations.
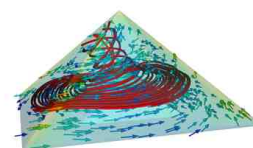
Hans Fangohr

Selected Upcoming Computational Physics Events

Condensed Matter and Materials Physics 2010

▷ 14 - 16 December 2010, Warwick University

▷ http://www.cmmp.org.uk/

CMMP10, 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.

Conference on Computational Physics Gatlinburg 2011 (CCP 2011)

▷ 16-20 October 2011

▷ Oak Ridge National Laboratory, Tennessee, US

Related Newsletters

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

▷ Newsletter of the Computational Physics Division of the American Physical Society:

http://www.aps.org/units/dcomp/newsletters/index.cfm

▷ Europhysicsnews newsletter of the European Physical Society (EPS):

http://www.europhysicsnews.org/

▷ Newsletter of the Psi-k (Ψ_k) network:

http://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:

http://www.industrialmath.net/content/news.

Computational Physics Group Committee

Michael Barnes	`michael.barnes@pysics.ox.ac.uk`
Peter Borcherds	`p.h.borcherds@birmingham.ac.uk`
Hans Fangohr (Newsletter)	`h.fangohr@soton.ac.uk`
Vera Hazelwood (Thesis prize)	`Vera.Hazelwood@smithinst.co.uk`
Andrew Horsfield (Treasurer)	`a.horsfield@imperial.ac.uk`
Paul Hulse	`paul.hulse@sellafieldsites.com`
Geraint Lewis (Chair)	`Geraint.Lewis4@wales.nhs.uk`
Ian Morrison	`i.morrison@salford.ac.uk`
John Pelan	`j.pelan@gatsby.ucl.ac.uk`
David Quigley	`d.quigley@warwick.ac.uk`
Jesus Rogel (Secretary)	`j.rogel@physics.org`
David Shipley	`david.shipley@npl.co.uk`
Nathan Sircombe	`Nathan.Sircombe@awe.co.uk`

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 Geraint Lewis.