

Newsletter

```
program average
! Read in some numbers and take the average
! As written, if there are no data points, an average of zero is returned
! While this may not be desired behavior, it keeps this example simple

implicit none
integer :: number_of_points
real, dimension(:), allocatable :: points
real :: average_points=0., positive_average=0., negative_average=0.

write (*,*) "Input number of points to average:"
read (*,*) number_of_points

allocate (points(number_of_points))
write (*,*) "Enter the points to average:"
read (*,*) points

! Take the average by summing points and dividing by number of points
if (number_of_points > 0) average_points = sum(points)/number_of_points

! Now form average over positive and negative points only
if (count(points > 0.) > 0) positive_average = sum(points, points > 0.) /
    count(points > 0.)
if (count(points < 0.) > 0) negative_average = sum(points, points < 0.) /
    count(points < 0.)

deallocate (points)

! Print result to terminal
write (*,*) "Average = ", lg124, average_points
write (*,*) "Average of positive points = ", lg124, positive_average
write (*,*) "Average of negative points = ", lg124, negative_average

end program average
```

The BCS Fortran Specialist Group

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Figure on cover:

A short Fortran programme taken from <http://en.wikipedia.org/wiki/Fortran>. See page 1 for the corresponding article.

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. Due to financial constraints, this edition is only distributed electronically.

The *main feature* (page 1) of this newsletter is an introduction to the BCS Fortran Specialist Group. Fortran is of course a major language in high performance computing, and actively developed.

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

The Computational Physics Group Committee.

Introducing the BCS Fortran Specialist Group

John Pelan, MInstP (vice-chairman of the FSG)

As many computational physicists know, despite occasional claims to the contrary, the **Fortran** programming language is alive and well. Aside from it being fit-for-purpose, much of its relative strength lies in the fact that as an open, international standard it provides a stable, portable language for the description of computational tasks. What many physicists may not know, is that the Fortran standard continues to develop at a pace and at the heart of much of this effort in the UK lies the **BCS Fortran Specialist Group**.

BCS is the “Chartered Institute for IT” [1] and, as with other professional bodies in the UK, is constituted and structured in a similar manner to the IoP. BCS’s stated aims are “to promote wider social and economic progress through the advancement of information technology science and practice”. There are over 70,000 members including practitioners, businesses, academics and students, in the UK and abroad. As it happens, BCS is currently undergoing a transformation exercise with a new logo and much promotional activity [2].

Like the IoP, BCS has a number of specialist groups. The Fortran Specialist Group (FSG) [3] was established in 1970 to provide an open forum for Fortran users. Our main aims are:

- ▷ to disseminate information about Fortran and its application in various fields
- ▷ to provide a platform for discussion of users’ needs and requirements in future versions of Fortran
- ▷ to encourage the development of the language in collaboration with national and international standardization bodies
- ▷ to promote the use of the Fortran language

Our group naturally organises events and meetings related to the Fortran language, with a particular emphasis on the Fortran standard - a perpetual endeavour. Amongst our committee members are John Reid and David Muxworthy, eminent in the standards activity. John Reid will also be familiar to many as one half of Metcalfe & Reid, authors of a series of seminal Fortran texts stretching back over twenty years. In 2007, we celebrated the 50th anniversary of the language with a one-day meeting in London [4]. There was a related article in the IoP’s very own **Physics World** co-authored by our chairman Peter Crouch, Clive Page and myself [5].

Current Developments

At present, the next standard, informally called **Fortran 2008**, is at “Final Committee Draft” stage. Under ISO procedures only editorial comments and clarifications may be made now unless a major technical defect is detected. All being well it will be

REFERENCES

ratified by an international vote and published by this time next year. We anticipate having some form of meeting to celebrate this milestone and to provide an exposition of the latest language features, expected to include explicit parallelism using coarrays. January will also be the 40th anniversary of the FSG.

We are also considering widening our remit to reflect the use of other computational languages and environments like python and Matlab, where historically Fortran would have dominated. This is not to abandon Fortran but to recognise that computational problems are often tackled at higher levels of abstraction, using purpose-built modules where the underlying source code is rarely or never seen. As it stands, it isn't always evident from reading the literature which scientific codes utilise Fortran exclusively or even partially. It has been suggested this visibility issue needs to be addressed particularly if the lack of apparent use of the language is discouraging its take-up by new students and graduates.

Getting Involved

Our meetings are usually free and open to all, with some provisos regarding pre-registration depending on the venue. They are advertised on our website and on the JISC Fortran mailing list [6]. We will undertake to notify the computational physics community of anything relevant via this newsletter and other channels where appropriate and it is hoped that the Computational Physics group and ourselves will host a joint event in the foreseeable future.

We are required by BCS to encourage membership, the entry level being that of Affiliate which is currently £36 per annum although you may find the benefits of full membership attractive. Full-time students can pay £40 which covers them for the duration of their course. Further details can be found on the BCS website [1].

References

- [1] <http://www.bcs.org>
- [2] <http://www.bcs.org/upload/pdf/transformation-update-sep09.pdf>
- [3] <http://www.fortran.bcs.org>
- [4] <http://www.fortran.bcs.org/2007/jubileeprog.php>
- [5] *"Fortran faces the future at 50"*, Crouch P, Page C and Pelan J; Physics World, Dec 2007 p31
- [6] <http://www.jiscmail.ac.uk/lists/comp-fortran-90.html>

Computational Physics Group News

Invitation to join

We are always looking for enthusiastic new members to join the Computational Physics Group Committee.

Committee Membership Benefits

- ▷ Meet like-minded colleagues in the field.
- ▷ Arrange (with the help of IoP) meetings of interest to you and others.
- ▷ Help shape IoP policy on Computational Physics.
- ▷ Widen contacts with the Computational Physics Group membership.

Commitments

Meetings are in London, 3 times per year, expenses reimbursed.

Requirements

Member of IoP and Computational Physics Group (which is free to IOP members).

Next steps

Email Geraint Lewis (Geraint.Lewis@velindre-tr.wales.nhs.uk) with an expression of interest.

The Computational Physics Thesis Prize 2008

The Winner of the Computational Physics Thesis Prize 2008 is Dr Vanessa de Souza (previously at the University of Cambridge, now at the University of Sydney, Australia) for her work on Glassy Dynamics and the Potential Energy Landscape. Congratulations!

The Computational Physics Thesis Prize 2009

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 £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 28th, 2010.
- ▷ 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 VERA HAZELWOOD
email: vera.hazelwood@smithinst.co.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 2009.

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.

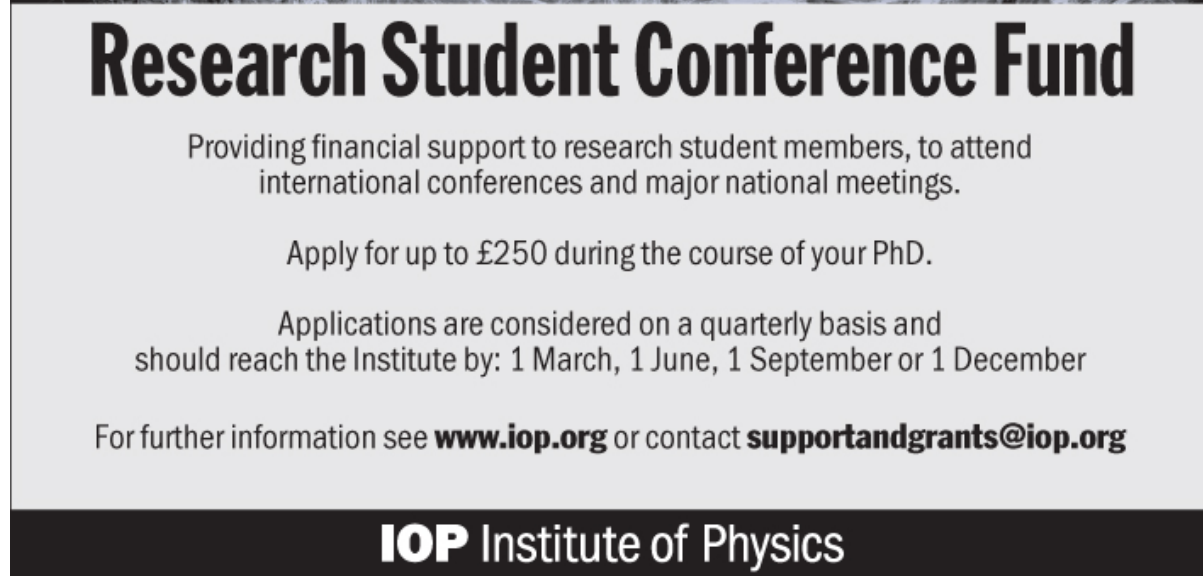
See <http://c20.iupap.org/prizes.htm> for details.

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.



Supporting research students



Research Student Conference Fund

Providing financial support to research student members, to attend international conferences and major national meetings.

Apply for up to £250 during the course of your PhD.

Applications are considered on a quarterly basis and should reach the Institute by: 1 March, 1 June, 1 September or 1 December

For further information see www.iop.org or contact supportandgrants@iop.org

IOP Institute of Physics

Further details can be found at

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

Reports on meetings

Particle Therapy, Technology and Clinical Applications

19 and 20 May 2009, British Institute of Radiology President's Conference 2009, London

This meeting was held at the British Institute of Radiology, London with well over 100 attendees. It was designed to showcase the present and future technology for particle-based radiotherapy (involving protons and other heavier ions such as carbon), and provide some clinical presentations of experience with the currently available technology. Day 1 focused on technology and clinical experience Day 2 took the discussion forwards with consider the role of carbon ions, imaging techniques to select patients for x-ray, proton and carbon ion therapy, and long-term consequences of radiotherapy Day 2 concluded with specific presentations of the UK position. The meeting was of interest to Medical Physicists, Radiotherapy Clinicians, Researchers in Particle and Nuclear Physics, Trust Managers and Oncology Managers .

Plasmas, Computation and Mathematics

18th-21st July 2009, Ambleside (UK)

38 participants from the UK, US, Germany, Portugal and Belgium met in Ambleside (Cumbria) to spend 4 days discussing diverse topics in the physics, computation and mathematics of plasmas. A broad range of stimulating talks (25 in total) was given, and of the 13 remaining participants 5 presented posters.

About half of the participants were early career researchers or PhD students. Round-table discussion sessions were held in a room near to the lecture theatre, which encouraged substantial dialogue between all of the participants. Approximately 30 minutes of discussion time was allocated to every 2.5 hours of talks, and everyone was given ample opportunity to join in. A friendly atmosphere was maintained throughout the workshop; students and senior researchers alike participated fully in the well-attended discussions.

The talks were split into 5 sessions :

- ▷ Magnetodynamics and Strong Field Interactions
- ▷ Magnetic and Inertial Confinement Fusion
- ▷ Beam-Plasma Instabilities
- ▷ Intense Laser-Plasma Interactions
- ▷ Astrophysical Plasmas

and included the following keynote presentations :

- ▷ Magnetohydrodynamic Relaxation To States Of Complex Topology, Keith Moffat FRS (Cambridge)
- ▷ Twisting and Sheared Flows In Tokamaks, Steve Cowley (Director, UKAEA)
- ▷ Fundamental Aspects Of Plasma Turbulence At Sub-Larmor Scales, Alex Schekochihin (Oxford)
- ▷ Blowing Bubbles: How Non-Stationary Plasma Structures Capture, Accelerate, And Improve Electron Beams In Laser Wakefield Accelerators, Gennady Shvets (Texas, Austin)
- ▷ Kinetic Plasma Modeling With Petascale Systems: Making Direct Contact Between Experiment And Simulation, Ricardo Fonseca (IST & ISCTE, Lisbon)
- ▷ Modeling Of Plasmas And Plasma Growth Of Carbon Nanostructured Materials, Erik Neyts (Antwerp)
- ▷ Cosmic Ray Acceleration, Tony Bell (Oxford & STFC CLF, RAL)

The participants enjoyed the breadth of topics covered by the meeting and were made aware of a number of different areas outside of their own research. Most people found the round-table discussion sessions very useful and commented that the friendly environment was highly conducive to useful discussion. The resounding success of the workshop was underlined by requests for it to be repeated in the future.

Computer Simulation and the Environment

Thursday, 10 September 2009, IoP Headquarters, London.

This was a meeting jointly organised by the Computational Physics Group and the Environmental physics Group. We had four talks about computer simulations and how to obtain sufficient computer power, and two talks from hardware vendors on what they have to offer. Getting people to attend was difficult (about 20 turned up) which was tricky because the vendors had quite high expectations.

European workshop on Monte Carlo Treatment Planning

19-21 October 2009, National Museum of Wales, Cardiff

The introduction into clinical practice of more accurate methods for patient dose calculation for cancer radiotherapy is of paramount importance. Algorithms based on the Monte Carlo (MC) method are widely regarded as the most accurate available. MC techniques are also ideal research and development tools increasingly used in emerging areas including, among others, functional imaging, and molecular targeted

radiotherapy. The number of publications reporting the use of MC in radiotherapy treatment planning (MCTP) has indeed increased exponentially in the last 25 years.

The aim of MCTP2009 was to create an opportunity and environment to facilitate the integration of research, development and clinical implementation of MC technology in medical radiation physics devoted to the diagnosis and treatment of cancer. The meeting itself was well attended (by over 140 delegates from around the world) and supported by commercial vendors as well as the research community. Initial feedback from attendees to the conference organisers has been very positive in terms of venue, organisation and scientific content.

See also <http://www.mctp2009.org/>.

Selected Upcoming Computational Physics Events

Conference on Computational Physics (CCP) 2009

- ▷ 15-19 December 2009, Kaohsiung, Taiwan
- ▷ Abstract submission deadline is 30 June 2009
- ▷ See <http://www.ccp2009.tw/> for details

CCP is the worlds largest conference on Computational Physics. It is an annual event, rotating between the continents of Asia-Australia, Europe-Africa, and North and South America. In previous Asia-Australia rotations, it graced: Gyeongju, Korea 2006, Beijing, China 2003, Brisbane, Australia 2000.

Scientists in any area of computational physics are welcome to participate. Sub-fields such as Condensed Matter, AMO, Plasma/Space, High Energy, QIS, Complex Systems, Education, New Method form the major program, Petaflop and GPU Super-computing.

Even in December, Taiwan has beautiful weather. The culture, cuisine and scenery will make the visit refreshing in addition to academic enriching.

Condensed Matter and Materials Physics (CMMP 09)

- ▷ 15 - 17 December 2009
- ▷ Warwick University, UK
- ▷ http://www.iop.org/Conferences/Forthcoming_Institute_Conferences/CMMP09/page_32870.html

The annual group meeting of the Computational Physics Group will take place at the CMMP 2009.

Monte Carlo Neutron, Electron and Gamma (MCNEG) 2010

- ▷ 12-13 April 2010
 - ▷ at National Physics Laboratory (NPL)
-

Conference on Computational Physics Trondheim 2010 (CCP 2010)

- ▷ 23-26 June 2010
- ▷ Trondheim, Norway
- ▷ <http://www.ccp2010.no><http://www.ccp2010.no>

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>.

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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.