

C20. Commission on Computational Physics

Report to the 2008 General Assembly for 2005-2008

Officers 2005-2008

Chairman: Peter Borchers UK
Vice Chairman: Jai Sam Kim Korea
Secretary: James Gubernatis USA

Members 2005-2008

Nithaya Chetty	South Africa
Hugh Couchman	Canada
Peter Drummond	Australia
Juergen Hafner	Austria
Alejandro Muramatsu	Germany
Ravil Nazirov	Russia
Yutaka Okabe	Japan
Amr Shaarawi	Egypt
Laszlo Szunyogh	Hungary
Shaoping Zhu	China

Associate Members 2005-2008

Jaroslav Nadrchal	Czech Republic
Jamie Shiers	Switzerland
Toshikazu Takada	Japan
Chris Wolverton	USA

1 Activities

Conferences:

C20 organises an annual conference under the generic name Conference on Computational Physics [CCP]. Our recent conferences have been

CCP2006 Gyeongju, South Korea
CCP2007 Brussels, Belgium

CCP2008 Ouro Preto, Brazil

All these conferences have been very successful.

C20 works closely with the Division of Computational Physics Division (DCOMP) of the American Physics Society (APS), with the Computational Physics Group of European Physical Society (EPS), and with the Association of Asian Pacific Physical Societies (AAPPS) in identifying conference organizers and promoting the conferences. The conferences are allocated to these bodies on a triennial cycle. The next conferences will be held in Taiwan [CCP2009] and Norway [CCP2010].

For further information on past conferences see the C20 web site:
<http://c20.iupap.org>

Prizes:

Since 2007 C20 has awarded the IUPAP Young Scientist Prize in Computational Physics. The prize winners have been:

2007	Stefan Sanvito	Ireland
2008	Naoki Yoshida	Japan

In all cases the prizewinner has given a lecture on the work for which the prize was awarded. This has been given at a special prize giving ceremony, which has been held at the end of the conference. We have found scheduling the ceremony at this time encourages delegates and conference attendees to remain until the end of the meeting.

The number of nominees tripled between the first and second award because of better advertising and the co-ordination of that advertising with associated physical societies. These two awards have quickly set a standard for future recipients.

When the CCP is held in Europe, the European Center for Atomic and Molecular Computations (CECAM) sponsors the prestigious Berni Alder Prize, named in honour of Berni Alder (Lawrence Livermore National Laboratory, USA) one of the pioneers of Computational Physics. The 2007 winner was Daan Frenkel from the Netherlands. The prize was presented by Berni Alder himself.

The Commission recently revised its procedure for nominations for this award. Initially, it adopted that from another commission. The new procedures should be a big step toward gathering more information to assist commission members in making more informed decisions. The actual and potential diversity of the scientific fields of the nominees was greater, and will likely always be greater, than that of the

commission members. Commissions are staffed on the basis of geographic and national diversity and not scientific diversity. Computational Physics is the broadest area of physics presently existing. The new procedure is posted on the Commission's website.

Meetings of the Commission:

Much of the business of the Commission has been done by email, e.g., the assessment of the entries for the Young Scientist Prize. Communication among the officers is often supplemented by telephone calls.

We have held 3 meetings, each in association with a CCP conference. The attendance has been disappointing, largely because Commission Members have difficulty in obtaining funding for travel to Commission Meetings. We believe that face-to-face meetings are very valuable, and suggest that National Liaison Committees be encouraged to obtain funding for Commission Members to take a more active part in Commission business. Face-to-face discussion of issues expedites their resolution. Such meetings also foster more rapport among commission members and develop in the Commission a better sense of computational physics in the host countries and the countries of the attendees.

2 Highlights in Computational Physics

A very striking aspect of Computational Physics follows from Moore's Law, which can be loosely interpreted as saying that in computing everything halves or doubles every 2 years: it is more dramatic to say everything changes by 1000 times every 20 years. 2008 is the 60th anniversary of the invention of the transistor, and we now have chips with a billion or more components on them.

In fact, advances in computational physics have been even more dramatic: an early example of this, circa 1965, was the development of the Fast Fourier Transform [FFT], where use of this software can lead to an increase of million fold or more in speed independent of any hardware developments. Recently, the Petaflop computing barrier was broken by the Roadrunner computer developed through a joint program of the Los Alamos National Laboratory (USA) and the IBM Corporation. Throughout the past decade there has been a staggering increase in the use of multi-processor computers, some with tens of thousands of processors, many very affordable and accessible to modestly-sized institutions and departments.

These progressions of computing power find application in diverse areas of physics. For example, in biophysics new understandings of the protein function, control, and design are emerging. In nanotechnology, the grail of materials by design is being

approach. Computational physics is an area where future growth is clearly foreseeable.

3 Strategic Goals for 2009-2012

Young Scientist Prize:

Revisiting the advertisement of the award to insure its accessibility worldwide is warranted. Have we done our best? Such advertising also adds prestige to the award. After the 2009 award, the nomination procedure should be revisited for adjustments, if any.

Conferences:

Long-range endorsements of conferences should continue. For 2011 and 2012 preliminary contacts have been made about holding the conference in the USA and Japan. Following up on these contacts should produce able organizers of exciting conferences. Conferences in the Americas have typically been less well attended than those in Europe and Asia-Pacific. The reasons are not well understood. Working with the 2011 organizers to improve attendance is an important task for the new Commission.

Member Participation:

Email response from some commission members is either never, almost never, spotty, or responsible. More of the latter needs fostering. How to do this is unclear. Care in the appointments to the commission is a starting point.

Peter Borchers (Chairman)
James Gubernatis (Secretary)