

Commission on Computational Physics (C20) **Final Report, 2008-2011**

As other IUPAP commissions, C20 principal activities are sponsoring conferences and awarding Young Scientist Prizes. Two other activities occupied this commission's attention. One was selecting a new publisher for the proceedings of its conferences. The other was initiating with the Commission on Development (C13) a 10-year, biennial series of African schools on computational physics. Each of these four activities is now summarized. The roster of Commission membership is appended. The Commission's web page is at <http://phycomp.technion.ac.il/~C20/index.html>.

Conferences

Each year the Commission sponsors an international conference on computational physics called the Conference on Computational Physics (CCP). The conference rotates geographically in turn from a location in the European/African region to the Americas and to the Asian/Pacific region.

For 2009, C20's meeting, CCP2009, was held in Kaohsiung, Taiwan, from December 16-19, and was organized by Prof. James J. Y. Hsu of the National Cheng Kung University. Sessions on quantum information science, condensed matter physics, nanoscience, plasma physics, soft matter, biophysics, statistical physics, and atomic and molecular orbital physics occurred. The meeting's website is <http://www.ccp2009.tw/>. The proceedings from the conference was published as Computer Physics Communications, vol. 182, issue 1 (2011)

C20's 2010 annual conference on computational physics (CCP2010) was held June 23-26 in Trondheim, Norway and was organized by Prof. Alex Hansen of the Norwegian University of Science and Technology. Topics of the sessions included high-energy physics, astrophysics/plasma physics, complex systems, biophysics, quantum phase transitions, supercomputing, computational physics education, and computational physics in the Third World. The meeting's website is at <http://www.ccp2010.no/>. The proceedings from the conference was published as Computer Physics Communications, vol. 182, issue 9 (2011).

CCP2011 was held October 30-November 3 in Gatlinburg, TN USA with Dr. Malcom Stocks of the Oak Ridge National Laboratory as the organizer. Topics included:

materials/condensed matter theory and nano-science, strongly correlated systems and quantum phase transitions, quantum chemistry and atomic physics, high energy physics, astrophysics and plasma physics, complex systems – chaos and statistical physics, climate modeling, biological physics and soft materials, supercomputing and computational physics teaching, plus computational physics and sustainable energy. The conference website is at <http://ccp2011.ornl.gov/>. The conference proceedings are scheduled to appear early next year.

CCP2012 will be held October 14-18, 2012 in Kobe, Japan with Dr. Hideki Takabe (Osaka University) as the organizer. The web site is at <http://www.ile.osaka-u.ac.jp/CCP2012/>. CCP2013 will be held in Moscow, Russia with Prof. Lev Shchur (Landau Institute in Chernogolovka) as the organizer. A proposal to hold CCP2015 in India has been received.

Young Scientist Prizes

The Commission awards the Young Scientist Prize yearly. Each receipt receives the certificate and medal at the commission's annual conference where the recipient presents a plenary lecture on the research which lead to the award.

The Commission established a policy requiring its conference organizers to invite its Young Scientist Prize recipients to be on the organizing committee of the CCP meetings for up to five years after their award. This policy starts with CCP 2012. The intent of this policy is to tie emerging leaders more strongly to commission activities.

We awarded our 2009 Young Scientist Prize to *Dr. Amada Barnard* (CSIRO Materials Science & Engineering, Australia) for her computational work on nano-materials.

Dr. Philipp Werner of the ETH (Switzerland) was the C20's 2010 Young Scientist Prize winner for his work on algorithms for quantum Monte Carlo.

C20's 2011 Young Scientist Prize was awarded to *Prof. Stefano Curtarolo* of Duke University (USA) for his work on high throughput combinatorial computational materials science and his development of thermodynamic models for nano-catalysts.

Conference Proceedings

The Commission entered an agreement with the Journal of Physics Conference Series of the Institute of Physics to publish of the proceedings of its future CCP meetings. Changes in the publishing industry make the arrangement in place for the publishing of our proceedings as a

special issue of a particular journal difficult for our conference organizers. The new arrangement shifts the proceedings to an on-line publication with no restriction on page length. Preliminary and plenary papers will once again be acceptable, and videos and computers program can now accompany the papers. Our conference organizers will serve as the editor of their meeting's proceedings, and the papers will still be refereed. The papers will be visible to such search engines as Google Scholar. Most importantly, the proceedings will now be freely accessible to anyone who has Internet access; that is, they will now be available to those whose institutions may not have a subscription to the journals published by the Institute of Physics. In return, the Institute of Physics will advertize our meetings as a banner on the web pages of its computationally oriented journals. The arrangement started with CCP 2011.

African School

C20 worked with C13 to obtain IUPAP's endorsement of a 10 year, biennial series of African computational physics schools. The school's theme is numerical methods for electronic structure calculations.

The first school was held in Muizenberg, South Africa July 19-30, 2010. Prof. Joubert (Witwatersrand) headed the local organizing committee. Prof. Nithaya Chetty (Pretoria), a C20 commission member, and Dr. Sandro Scandolo (ICTP), a C13 commission member, provided key organization skills. Prof. R. M. Martin (UIUC/Stanford) heads the school's International Advisory Panel.

The website for the 2010 school is <http://asesma.ictp.it>. It was a huge success and has since been the subject of a commentary in Nature Physics and Physics Today, and the organizers have been asked to write a review of its activities for the Newsletter of the National Society of Black Physicists (USA). Appended is a brief report of the school's activities.

The 2012 school will be in Eldoret, Kenya during June 2012. Profs. George Amolo and Nicholas Makau (Moi University) will head the local organization.

Commission Membership

Officers:

Chair: James Gubernatis (2008) (2005) (2002), Los Alamos National Laboratory (USA)

Vice-Chair: Peter Borchers (2008) (2005) (2002), University of Birmingham (UK)

Secretary: Yutaka Okabe* (2008) (2005), Tokyo Metropolitan University (Japan)

Members:

Joan Adler (2008), Technion, Israel Institute of Technology (Israel)

Nithaya Chetty (2008) (2005), University of Pretoria (South Africa)

Giovanni Ciccotti (2008), Università degli Studi di Roma "La Sapienza" (Italy)

Hugh Couchman (2008) (2005), McMaster University (Canada)

Guang-Yu Guo (2008), National Taiwan University (China-Taipei)

Alex Hansen (2008) (2005), Norwegian University of Science and Technology (Norway)

Joaquin Marro (2008), University of Granada (Spain)

Alejandro Muramatsu (2008) (2005), Universität Stuttgart (Germany)

Ravil Nazirov* (2008) (2005), Space Research Institute, Russian Academy of Sciences (Russia)

Jian-Sheng Wang (2008), National University of Singapore (Singapore)

Tony Williams (2008), University of Adelaide (Australia)

Associate Members: 2009 - 2012

Constantia Alexandrou (from C12), University of Cyprus (Cyprus)

Richard M. Martin, University of Illinois, Urbana-Champaign (USA)

Jean-Paul Ryckaert, L'Université Libre de Bruxelles (Belgium)

Hideaki (Aki) Takabe, Osaka University (Japan)

* Inactive

**African School on Electronic Structure Methods and Applications (ASESMA)
Muizenberg, Cape Town 19- 30 July 2010.**

The inaugural school in the biennial series planned for 2010-2020

Summary of the ongoing activities of ASESMA

ASESMA-2010 was not just a two week school. It was the start of an ongoing network for interaction and collaboration. By all accounts, it was a fantastic success. The participants are continuing to stay in touch in 2011 long after the school. Several have started studies made possible by contacts made at the school, and there is enthusiasm for the future, and several others have gone to meetings in Europe through contacts made at the school.

* Much of the success of the school was due to an innovative program of mentors. The mentors are motivated young scientists mainly at the post-doctoral level, who worked with the participants one-on-one throughout the school. Since the school they have contacted every student; have on-going email communications advising on science and computing issues; set up web pages, a monthly electronic newsletter, and a Facebook page. (Links are given below). The participants, mentors and lecturers are enthused and the test will be the extent to which the interactions and collaborations continue into the future.

* The 2010 school was made possible by support of many international agencies:

* Support by the **International Union of Pure and Applied Physics (IUPAP)**, especially C13 and C20 commissions, was essential for international recognition of the series and for financial support of the 2010 School.

* A key role was played by the **International Centre for Theoretical Physics (ICTP) in Trieste**. Without their financial support the school could not have occurred. Probably more important were the scientists from Trieste, the ICTP, **Democratis Italian Simulation Center**, for their tremendous efforts at facilitating the use and easy access of the excellent Quantum Espresso codes, for making these freely available, and for coordinating the lectures.

* The South African Institute of Physics provided financial and administrative support. Further sponsors included The National Institute for Theoretical Physics in South Africa, the SA National Research Foundation, The Division of Computational Physics of the American Physical Society, and the Materials Computation Centre at the University of Illinois. The University of Witwatersrand offered a bursary for postgraduate studies at its Centre of Excellence in Strong Materials to the best performing participant at the School.

* The mentors were funded by the **International Center for Materials Research (ICMR) in Santa Barbara** with strong support by Prof. Nicola Spaldin. The mentor program was the innovation that helped students on a one-on-one basis. This helped improve the pace of the delivery as the participants were able to work independently. Each participant was able to progress based on his/her own abilities.

* There has been significant international coverage of the school and series including:

A commentary published in Nature Physics, 6, 1 (2010). A copy is available at:

<https://netfiles.uiuc.edu/rmartin/www/2010-ASESMA-Nature-Phys-nphys1842.pdf>

A report in Physics Today – “Raising the scientific level and networking in Africa”, by Toni Feder. Phys. Today 64, 28 (2011) A copy is available at:

<https://netfiles.uiuc.edu/rmartin/www/Phys-Today-ASESMA-PTO000028.pdf>

* A description of the ASESMA series can be found at

<https://netfiles.uiuc.edu/rmartin/www/AfricanSchoolSeries-rev-7-6.pdf>

This includes the international advisory board that consists of outstanding scientists.

* The websites and groups for ASESMA:

<http://asesma.ictp.it>

* A facebook page has been established

<http://www.facebook.com/?ref=logo#!/group.php?gid=145558648789192>

* A portrait gallery with contact information has been created.

<https://sites.google.com/site/asesma2010/>

* The 2012 school will be held at Moi University, Eldoret, Kenya, organized by George Amolo and Nicholas Makau. Efforts are underway to obtain support for participants and lecturers. IUPAP has committed to sponsor the series but financial support must be requested for each school. The ICTP has committed support for the 2012 school.

Report on the 2010 School in Muizenberg, Cape Town 19- 30 July 2010.

* Directors: Nithaya Chetty (University of Pretoria, South Africa), Richard Martin (University of Illinois, USA) Sandro Scandolo (International Centre for Theoretical Physics, Trieste, Italy)

Lecturers: Stefano deGironcoli, Paolo Giannozzi, Nicola Marzari, Shobhana Narasimhan, Renata Wentzcovitch, Phuti Ngoepe

Mentors: Tesfaye Abteu, Kris Delaney, Sinead Griffin, Allison Hatt, Amy Lazicki, Brice Malonda

* At the 2010 School there were 45 participants (in addition to the 6 mentors) from many countries in Africa: Cameroon, Congo, Ghana, Ethiopia, Kenya, Nigeria, South Africa and Zimbabwe. Many of the South African students were actually nationals from other African countries, so the school served a large number of graduate students and young faculty. (See photograph below.)

* The School schedule can be found at <http://users.aims.ac.za/~sandro/>, which includes a link to the School photos.

* The topic of the Series of Schools is theory and computational methods for predicting and understanding

properties of materials through calculations at the fundamental level of electronic structure. This is a growing field in which scientists with limited resources can have a large impact. A personal workstation is sufficient for many problems and the internet is making possible productive use of large computational facilities. It is within reach to create electronic structure community in Africa working at the level of forefront international research.

* The content of the 2010 School was a combination of theoretical background and hands-on calculations using workstations. Each student learned to install and use Linux codes, and the primary code for calculations was Quantum Espresso. Every student ran a calculation at the Centre for High Performance Computing in Cape Town, a facility meant for all Africans. A great effort was made to have coordinated talks on theory, computation, and on phase transitions under pressure, a not-so-simple example of problems in minerals and geophysics. The CHPC management invited each participant to apply for a user account which they can use from their home countries.

* The Centre for High Performance Computing in Cape Town has given all participants of the School access to their Blue Gene, which was donated by the IBM for African collaborations. The QE computations and collaborations could well be the first truly African-wide research activity on this facility.

* The African Institute for Mathematical Sciences (AIMS) provided a fantastic venue and backdrop for the hosting for ASESMA2010. The accommodation, catering, lecturing and computing facilities are excellent. For your information, the Canadian government has recently donated Can\$20m for the establishment of a network of AIMS centres in Africa that will include Ghana, Nigeria, Senegal, Ethiopia and South Africa, which is excellent news.

* There was excellent administrative support for the School by Milena Poropat (ICTP) and Linette White (South African Institute of Physics).

Richard Martin
Nithaya Chetty
Sandro Scandolo

Photograph of the participants, mentors, and lecturers:

