

C20 Activities  
J.E. Gubernatis, 10/01/2010

C20's principal activities are the yearly endorsement of an international conference and the yearly awarding of a Young Scientist Prize. This year it also helped start a series of African schools in computational physics. In this reporting year, two of C20's conferences occurred.

The Commission's 2009 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/>.

C20's 2010 meeting 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 <http://www.ccp2010.no/>.

CCP2011 will be held October 16-20 in Gatlinburg, TN USA with Dr. Malcom Stocks (Oak Ridge National Laboratory) as the organizer, CCP2012 will be held in Kobe, Japan with Dr. Hideki Takabe (Osaka University) as the organizer, and CCP2013 will be held in Moscow, Russia with Prof. Lev Shchur (Scientific Center in Chernogolovka) as the organizer.

The Commission awarded its 2009 Young Scientist Prize to Dr. Amada Barnard of Australia for computational work on nanomaterials. She received her award at CCP2009. Dr. Philipp Werner of the ETH, Switzerland was the Commission's 2010 Young Scientist Prizewinner for his work on algorithms for quantum Monte Carlo. He received his award at CCP2010.

C20 worked with C13 to obtain IUPAP's endorsement of a biennial series of African computational physics schools. C10 and C14 also endorsed this school. The school's theme will be numerical methods for electronic structure calculations. The first school was in Muizenberg, South Africa July 19-30. Prof. Joubert (Witwatersrand) headed the local organizing committee. Prof. Nithaya Chetty (Pretoria), C20 commission member, and Dr. Sandro Scandolo (ICTP), C13 commission member, provided key organization skills. Prof. R. M. Martin (UIUC/Stanford) heads the school's International Advisory Panel. The website for this year's school is <http://www.nithec.ac.za/general/10.php>. It was a huge success. The 2010 school will soon be the subject of a commentary in Nature Physics. The location of the 2012 school will be announced soon. Attached is a brief report of the schools activities, drafted by the organizers.

The commission entered agreement with the Journal of Physics Conference series of the Institute of Physics for it to be the publisher of the proceedings of future CCP meetings. The proceedings will now be freely accessible to anyone who has Internet access.

The commission's web page is at <http://c20.iupap.org/>.

**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**

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. Much of the enthusiasm of the students was due to an innovative program of mentors, 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 each, set up web pages, a monthly electronic newsletter (two editions have been posted), and a Facebook page. Links are given below. The participants, mentors and lecturers are enthused and now is the real test – to keep the interactions and collaborations going into the future.

\* There is also enthusiasm for the continuing Series of Schools. An illustrious International Advisory Panel will help the Series stay focused and active. Several countries are possibilities for the hosting the site for the 2012 school, and the choice will be made soon.

\* 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 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 and 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 a 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 range of international experts who lectured at the School was impressive. The School schedule can be found at <http://users.aims.ac.za/~sandro/>, which includes a link to the School photos.

\* Support by IUPAP, especially the 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 in Trieste. Without their financial support the school could not have occurred. Probably more important were the scientists from Trieste, the ICTP, Democritus 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 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 was excellent administrative support for the School by Milena Poropat (ICTP) and Linette White (South African Institute of Physics).

\* 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 of 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.

The next steps:

\* Some participants have projects to work on, and are exploring ways in which Quantum Espresso can be used in their current work. Others are exploring new projects, and the networking and further mentoring and support will assist to accomplish this.

\* Networking and continuing with the work and projects post-School is now a critical issue. A monthly electronic newsletter is underway coordinated by Alison Hatt (ICMR, Santa Barbara) has agreed to act as editor.

\* A more permanent website is being set up, hosted by the ICTP. The current School website is located at <http://www.nithec.ac.za/>

\* 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/>

\* Nature Physics has agreed to publish a 2000 word commentary on the School.

\* We are analysing questionnaires and feedback forms from the participants to help us improve on future Schools, and to understand better the needs for Africa.

\* The venue for the 2012 School will be announced by Richard Martin, the chair of the IAP. A number of countries are currently bidding to host the School. Securing further international funds for the 2012 School will be an important challenge for these next two years, and we will count on your assistance in this regard.

There is still a long journey ahead, but the 2010 School has made an excellent start, and the foundations are in place for us to build for the future. Creating an internationally credible electronic structure community in Africa is within our reach. The consequences of this will be extremely important for the development of science in Africa.

Nithaya Chetty (University of Pretoria, South Africa)

Richard Martin (University of Illinois, USA)

Sandro Scandolo (International Centre for Theoretical Physics, Trieste, Italy)

