Networking at the heart of African workshop on computational materials science

Alison Hatt

Arguably, African scientists have everything they need to do world-class computational materials science. Powerful electronic structure codes are shared freely on the web and resources like the South African Center for High Performance Computing offer bountiful CPU-hours with minimal hassle. All one needs, then, is a computer with an Internet connection and somewhere to plug it in, requirements almost every African university can meet.

"In principle you could be sitting on the top of Mt. Kilimanjaro doing world-class science," said Nithaya Chetty, Professor of Physics at the University of Pretoria in South Africa. "There's really no excuse."

But of course, it's not that simple. More fundamental than even funding and facilities is the need for knowledge-sharing and networking. Addressing these missing ingredients is the goal of the African School on Electronic Structure Methods and Applications.

Better known by its acronym, ASESMA offers a series of short schools teaching the theory and application of electronic structure methods every other summer in locations across Africa. The first school took place in 2010 in Cape Town, South Africa, as did the precursor school in 2008, which started the program rolling. Last summer, Chepkoilel University College, Eldoret, hosted the second ASESMA school up in the sunny highlands of northwestern Kenya, organized locally by professors George Amolo and Nicholas Makau.

The seeds for ASESMA were sown decades ago during late-into-the-night conversations between Chetty and his PhD adviser Richard Martin at the University of Illinois at Urbana-Champaign. Chetty arrived in Urbana-Champaign on a Fullbright Fellowship, in the midst of an improbable academic trajectory from a rural schoolhouse in apartheid South Africa to an esteemed professorship and high-ranking office at the National Research Foundation. He became Martin's first graduate student, and the two discovered a shared interest in the power of science and education to improve lives in the developing world.

Chetty and Martin created ASESMA in collaboration with Sandro Scandolo of the International Center for Theoretical Physics (ICTP) in Trieste, Italy. The two-week schools focus on Quantum ESPRESSO, a popular, open-source software package for electronic structure calculations, and include equal parts classroom lectures and hands-on computer labs. Students and teachers take all their meals together along with several daily coffee breaks, giving them ample time to network and discuss research ideas.

Most of the ASESMA students in Eldoret last summer were graduate students and early-career researchers. They arrived from every corner of the continent: Nigeria, Ethiopia, Congo, Cameroon, South Africa, Zimbabwe, Ghana, Tanzania, and Kenya were all represented.

Some were advanced students from the 2010 workshop who returned to hone their skills. In the intervening years, several of them had started PhD programs and traveled for foreign research visits following connections made at the previous school. They reunited like old friends and formed a sort of senior class within

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African School on Electronic Structure Methods and Applications

Sponsors and Endorsements

- American Physical Society Division of Computational Physics
- Democritos Centre
- International Center for Materials Research (ICMR) at the University of California, Santa Barbara
- International Centre for Theoretical Physics in Trieste, Italy
- International Union for Pure and Applied Physics (IUPAP) Commissions (Physics Development, Computational Physics, Physics Education, and Structure and Dynamics of Condensed Matter)
- National Institute for Theoretical Physics in South Africa
- National Research Foundation
- South African Institute of Physics
- University of Illinois at Urbana-Champaign Materials Computation Center
- University of Witwatersrand Centre of Excellence in Strong Materials

the school, sharing their expertise with the new students.

Others were recent transplants to the field, like Calvince Nyaruanda, a local PhD student who came to ASESMA for a crash-course on computational methods. Nyaruanda abandoned experimental research to avoid inadequate safety equipment in his underfunded lab and relished the expert introduction to his new field.

Annie Waketa, from the University of Duala, Cameroon, also came to ASESMA in the midst of a career change. Waketa did her PhD and postgraduate work in Europe, studying electron correlation in low-dimensional systems. Back then, the primary application she had in mind was quantum computing. On returning to Cameroon for a faculty position, Waketa realized that even if she had the necessary funding for such experiments, quantum computing seemed less relevant in the developing world. Now Waketa is building an affordable and practical research program using electronic structure methods to develop materials for an inexpensive, African-made solar cell. Inspired by the success of the Eldoret school, Waketa is now working with Bernard M'Passi Mabiala, a professor from the Congo, to form an ASESMA regional working group.

Differentiating ASESMA from similar programs worldwide is the inclusion of mentors: advanced students and postdocs who assist with tutorials and provide a critical link between students and teachers. The mentors at the first school hailed mainly from the United States and Western Europe, as did the international bevy of lecturers, but they forged close connections with the African participants and proved to be an indispensable ingredient.

"Having mentors and tutors at the workshop is really unique," said Martin, when I spoke to him between lectures in Eldoret. "ASESMA 2010 was the first time I'd seen it at a school and it was just remarkably successful. And this year the mentors are mainly African students from 2010, which points to the success of the previous school."

The mentors are encouraged to stay in touch with the students long after the school, which helps promote another vital element of the program: community. Between schools, ASESMA remains active. The organizers encourage and facilitate collaboration between participants and lecturers, and between 2010 and 2012 workshops, ASESMA funding supported several research visits for former students. A regular newsletter and an active Facebook group help keep ASESMA members in touch and provide a sense of community.

This growing electronic structure community in Africa may prove to be the greatest legacy of the ASESMA program, as it addresses one of the biggest challenges facing African scientists. Speaking to the participants in Eldoret, the most common complaint I heard was of isolation. It appears that Africans are good at making the most of limited resources, but overcoming isolation takes more than resourcefulness.

Makau said, "After the school, if you go back to your country and you're alone and you don't know who is doing what where, then you don't make progress. So one of the things that is very important is to form networks. If you're in a network then you know what people are working on; if you have a problem you can contact someone."

There can also be a sense of alienation for African scientists due to the huge discrepancy between the academic world they are trying to engage and the society around them. According to Waketa, "Scientists here feel really out of phase with our daily environment. We feel like extraterrestrials, disconnected from reality."

And at its most basic, the isolation is about access to fresh ideas and collaboration. Martin said, "Science works that way in every country. The stimulation of working with people at the forefront is what makes science work in America

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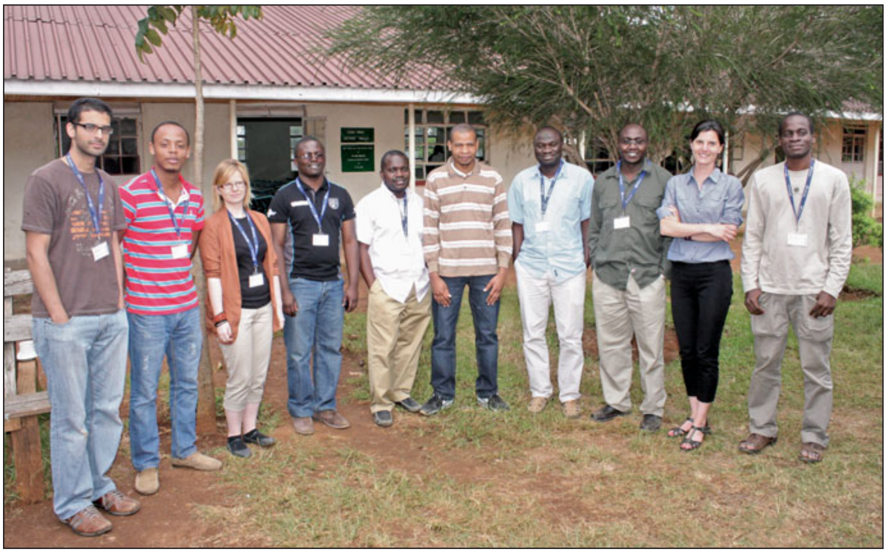

or Western Europe and that's exactly the same case here."

Western scientists have been engaging with Africa for decades, but ASESMA represents a new approach to promoting science education on the continent. "In the past, the mode of engagement largely involved a sprinkling of African scientists going over to Western destinations," said Chetty. "And as a result of that there's now a sprinkling of good scientists at institutions across Africa. But the real difficulty now is to assist those individuals to establish themselves in their local environments, to ensure that they're not totally isolated, that they continue to develop and grow the next cohort of students and researchers. And the way to do that is to have Western scientists travel to Africa."

By bringing the ASESMA lecturers to Africa, Chetty hopes to accelerate the dissemination of knowledge, as a single lecturer can have an impact on 60 students instead of just one. But Chetty also wants something more: to educate the Western world about the state of science in Africa. In a program like ASESMA, Chetty said, "Don't think we're starting from level zero. That's the message I'd like to get across to countries like the USA and Western Europe."

Scandolo agrees. "That's also one of the purposes of ASESMA: to bring lecturers from Western countries to Africa and get them to see how people work here, that there is science being done in these places in spite of the sometimes difficult conditions, lack of research funds, and so on."

This reverse education may help answer a common question in Western minds: Why do computational materials research in a place where so many other problems—poverty, hunger, human rights to name a few—are pressing?

Chetty summed it up for me: "Africa has a lot of serious problems and we cannot ignore that. We have problems of poverty and war-stricken areas and food security and epidemic diseases of enormous magnitude like HIV AIDS and so on. The pressing problems need to be addressed politically and there need to be short-term efforts to relieve African countries of those problems. I don't think electronic structure calculations will be doing that in the short term. But in the long term, make no mistake about what science will be doing or has the potential to do in terms of addressing those problems.

"Programs like ASESMA might seem insignificant, and yes the impact we make here is just a drop in the bucket, but it's an impact nonetheless. Eventually these things do add up."

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