The Growth of High-Performance Computing in Africa

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Much of Africa has limited experimental research facilities in many areas of fundamental and applied sciences. There are, however, cases where government support has made a difference in providing both infrastructure and funding to researchers as well as graduate students to carry out experimental work. This article describes continent-wide initiatives to grow computational sciences and high-performance computing work. These programs are expected to produce African researchers and scholars who will drive the materials science research agenda, thereby directly influencing their own economies.

A large part of Africa is limited in both basic and advanced experimental research facilities that can consistently be used by faculty to perform studies in many areas of fundamental and applied sciences. In cases where such facilities exist, the cost of maintenance is prohibitive, leading to long periods of inactivity due to lack of spare parts, and eventually abandonment in many cases. There are, however, cases in South Africa where government support has made a difference in providing both infrastructure and funding to researchers as well as graduate students to carry out experimental work. A majority of African governments would appreciate visible short term impacts of investment in research but with less consideration for continual support to grow capacity among youth and upcoming young researchers.

The ability to perform good science using computer codes[1–3] founded on the fundamental sciences[4–6] is an avenue for scientists and engineers to stay active and professionally fulfilled through involvement in research within the developing world as well as with collaborators abroad. The recent evolution of affordable computers with reasonably sized RAM and storage capacity makes computational science attractive to developing nations, especially those with active groups as well as basic support from local institutions and their respective governments. Computational science is now being widely applied in areas such as materials science, drug design, astronomy, and business intelligence. In basic science subjects such as physics, as well as chemistry and, very recently, biology, the availability of open source 3D state-of-the-art visualization programs has greatly boosted the level of appreciation and understanding of structures

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with sizes ranging from a few to several tens of atoms/molecules. In the past, learners had to contend with 2D static structures on text books or enlarged pictures on chart illustrations.

While calculations of small systems might be done on stand-alone computers, medium- to large-sized systems require the use of high performance computing (HPC) facilities. The largest support of HPC in Africa has been provided by the Centre for High Performance Computing (CHPC) in Cape Town, South Africa.[7] To access these facilities, the CHPC requires African researchers or academics to register as principal investigators under various research themes. Registered graduate students are encouraged to work under the relevant research themes available.

Figure 1. Participants at the opening ceremonies of the fourth African School on Electronic Structure Methods and Applications (ASESMA), which was held at the University of Ghana, 11–25 June 2016.

CONTINENT-WIDE INITIATIVES TO GROW COMPUTATIONAL SCIENCES AND HPC

The African School on Electronic Structure Methods and Applications (ASESMA) is an initiative to introduce computational modeling to African academia, researchers as well as graduate students.[8] It started in 2008, with the first meeting held in Cape Town, South Africa. The ASESMA series are planned to be biannual, and have already been held in 2010, 2012, 2015, and 2016. It is expected that these series will run until 2020. The 2010 series was held in Cape Town, with those in 2012, 2015 and 2016 taking place in Eldoret (Kenya), Johannesburg (South Africa), and Accra (Ghana), respectively.[9] The initial focus was on materials science, with physics and chemistry as the fundamental subjects, but has grown to involve biological systems and applied sciences such as materials engineering. The CHPC now has a much larger user base that includes drug design and astronomy, among others.

The CHPC has provided computational resources and temporary storage to ASESMA participants during the various schools held in the African continent. CHPC's contribution as well as the continued support of the South African government are highly acknowledged. ASESMA, whose activities have resulted in the training of one of the largest groups of African scholars in materials science, has enjoyed the support and sponsorship of several host African governments and international institutions. Figure 1 show a group photo of the fourth ASESMA event, held at the University of Ghana in 2016.

There are regional initiatives by groups in various parts of Africa that have, through their own governmental resources and support from international institutions, set up small HPC facilities that have enabled local researchers and graduate students to engage in simulations of materials of interest. Computational science groups in Ethiopia, Ghana, Kenya, and Zambia have small HPC facilities that have been set up mainly by local resources. The HPC facility in the Sudan was set up with the support of the Chinese government. In Kenya, the Kenya Education Network (KENET)[10] is supporting a special interest group, Computational Modeling and Materials Science, by facilitating workshops on the use of HPC resources as well as on proposal writing to prepare members to compete for local and international research grants. Figure 2 shows a group photo of the participants during a recent workshop on proposal preparation on themes related to computational sciences.

Figure 2. Participants of a recent Kenya Education Network (KENET) sponsored workshop in Kenya on the use of HPC facilities and competitive proposal preparation for local and international grants.

OUTCOMES AND EXPECTED IMPACTS OF THE USE OF HPC FACILITIES

To date, the ASESMA initiative has opened training opportunities to tens of graduate students who have obtained their masters and doctorates from universities in other parts of Africa and in Europe and taken up jobs as postdoctoral fellows in research institutions and as faculty members in universities.[11,12] Many of those who left their countries of origin have returned home and secured employment in universities, government departments, and the private sector. It is noteworthy that many of them have attracted new students, indeed creating their own groups to continue with research.

CONCLUSIONS

The use of HPC to simulate real and large systems is important for the advancement of science in general. Simulations can not only independently reproduce known properties of materials but can also predict the existence of new materials phases and properties not accessible to experimental work, hence acting as a vital decision support tool. Access to HPC resources to support strategic and focused experimental research might be key to Africa's growth in an effort to diversify revenue generation from the already saturated and traditional economic bases of agriculture and tourism to manufacturing of products for local consumption, hence creating employment opportunities for youth in the long term.

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