Computational Science in Developing Countries
Recognizing Excellence in High Performance Computing

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This special CiSE issue offers comments and thoughts about computational science in developing countries. Several successful national and international initiatives concerning high-performance computing education and training are described. In addition to countries officially classified as developing, programs for underprivileged minorities in mostly developed countries are also mentioned.

There has been much discussion of “What is computational science?” in this magazine; this is indeed an important topic, and its distinction from core computer science can be confusing. For this current issue of CiSE, the quandary is “What is a developing country?” Since 2016, the World Bank has dropped the developed/developing distinction, so we chose as a first approximation the International Statistical Institute (ISI) list, which is based on World Bank data (www.isi-web.org/index.php/resources/developing-countries).

Decisions concerning which countries are “developed” lead to some absurdities. Countries with representatives in the June 2017 Top500 computer list (www.top500.org) include several that also feature in the developing country list and host projects described in this issue. One extreme is China, which had the top two computers in the November 2017 Top500 list but is classified as developing. The other extreme is Israel, which currently has no computers in this ranking (and has historically had very few, and never any in high positions) but is considered developed and has a highly developed hardware and software industry. Some countries officially classified as developing have average low incomes but an outstanding record of scientific research and education, for example, the Russian Federation.

An aspect related to our topic is computational science development for underprivileged minorities within otherwise developed countries. These range from township black children in South Africa to native Americans in the US and minority populations in countries such as Israel and India. Although not intentionally excluding projects concerning encouragement of women in science and engineering in both developed and developing countries, our emphasis has been on gender-neutral projects.

A seminal organization for physics in developing countries is the International Center for Theoretical Physics (ICTP; www.ictp.it) in Trieste, Italy. Funded by Nobel Prize Laureate Abdus Salam in 1964, it’s played a role in the African School on Electronic Structure Methods and Applications (ASESMA) project, which is reviewed in this issue. The center is not limited to theoretical physics; its early adoption of Linux and parallel computing has supported computational advances in the developing world.
Another ASESMA sponsor is a subcommission of the International Commission for Pure and Applied Physics (IUPAP): C13 Physics for Development, which was established in 1981 (iu-pap.org/commissions/c13-physics-for-development).

There has also been general engineering and high-performance computing (HPC) activity in developing countries, although most is relatively recent compared to ICTP. In the more general computational science area, the EU has sponsored projects—most notably LinkSCEEM (described in detail in this issue), which includes EU-associated countries clearly classed as developing, and RISC, which served as the initial link between several countries in South America and Europe. A current HPC continent-wide initiative has been selected for detailed discussion. (Figure 1 highlights just one of the many current activities supporting this effort.)

A complicating factor is that the criterion of per capita income used to distinguish developed/developing varies greatly within countries. The EU, US National Science Foundation, and other funding bodies have special programs for minorities. One example is the Israeli Science Ministry projects for Arab, Druse, and Circassian students, and new immigrants from Ethiopia (www.gov.il/he). Some of these require special attention due to different languages of instruction. At the Technion, we have many Arab (Christian and Muslim) as well as Druse students, many of whom wear traditional dress to class. (Figure 2 features two Technion students who are members of a minority community.)

Computational science has played an enormous role in many of the Asian “tiger” economies; countries such as Singapore and China have become leaders in this area in recent years, with both HPC centers and research activity. Some of these countries are now classified as developed and have not been emphasized in detail in this issue.
Figure 2. Joan Adler (left) with two students from her computational physics class whose project connected Wolfgang Christian's phsylet applets to the Israeli high school syllabus, with instructions for their use by high school teachers.

Two of the projects highlighted in this special CiSE issue encourage use of HPC, visualization, and advanced algorithms by students and researchers who have not been previously exposed to serious research or computing. It would be impossible to mention all of the computational science initiatives in only one collection of articles, and so our selection was arbitrary—with apologies to those who were not invited or exposed to our calls. Descriptions of good educational projects in computational science are welcome to be submitted to CiSE as regular feature articles, and we hope that this issue will encourage such submissions.

ABOUT THE AUTHORS

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Linking Scientific Computing in Europe and the Eastern Mediterranean (LinkSCEEM) was an FP7 infrastructure project that established a high-performance computing (HPC) ecosystem in the Eastern Mediterranean region by interlinking and coordinating regional compute resources to form an integrated e-Infrastructure. The overarching objective of LinkSCEEM was to enable scientific research in the region by engaging and supporting research communities, with an initial emphasis in the fields of climate research, digital cultural heritage, and synchrotron radiation applications.

The FP7 infrastructure project Linking Scientific Computing in Europe and the Eastern Mediterranean (LinkSCEEM) established a high-performance computing (HPC) ecosystem in the Eastern Mediterranean region by interlinking and coordinating regional compute resources to form an integrated e-Infrastructure. It was the follow-up project to a coordination and support action that preceded LinkSCEEM. The coordinating institution was the Computation-based Science and Technology Research Center (CaSToRC) of the Cyprus Institute (CyI), with partners from Cyprus (CYNET), Egypt (BA and NARSS), France (ESRF), Germany (FZJ/JSC and MPG), Israel (Iucc), Jordan (SESAME and JUNET), and the US (NCSA).

LinkSCEEM’s overarching objective was to enable scientific research in the region by engaging and supporting research communities, with an initial emphasis in the fields of climate research, digital cultural heritage, and synchrotron radiation applications. To achieve its mission, LinkSCEEM adopted the following three-fold approach:

- Optimally integrate computational resources contributed by HPC centers in the Eastern Mediterranean region while establishing links with leading HPC centers and thus developing and sharing best practices for managing these resources.
- Create user support and training programs, in parallel to an active networking process that engages and integrates research communities and enables scientists in the region to...
utilize HPC for addressing complex scientific and engineering problems, thereby diminishing the digital divide.

- Develop a subset of HPC applications of particular relevance to the region—namely climate science, cultural heritage, and synchrotron radiation applications—and provide the links to leading groups in these fields to enable research of the highest standing. Thanks to the participation of world-leading HPC centers and research teams, core expertise of the highest level was introduced to the region both in the service provided and the spectrum of research enabled.

In summary, the main objectives of this project were to interlink and coordinate regional computational resources to form an integrated e-Infrastructure, as well as to provide the associated training activities and user support, engaging regional communities through networking activities such as workshops, exchange of visitors, organization of joint events, and outreach. This contributed to the creation of an HPC ecosystem from the individual group cluster to the Teraflop scale machines provided by CaSToRC and Bibliotheca Alexandrina (BA), and promoted the coordination of practices and methodologies.

The specific objectives of the project were as follows:

- **Objective 1:** Promote the establishment of user communities in computational science in the Eastern Mediterranean.
- **Objective 2:** Establish a resource allocation mechanism to coordinate access to the integrated simulation platform and its usage for research.
- **Objective 3:** Provide adequate training programs.
- **Objective 4:** Develop a dissemination and outreach program to publicize the project to the HPC and computational science communities in Europe and the Eastern Mediterranean. The program included the organization of an international conference, a continuously updated website, and focused outreach programs for computational scientists.
- **Objective 5:** Provide adequate user support.
- **Objective 6:** Adapt and develop software to support the optimization of parallel applications, data management, and visualization tools: (a) provide advanced user support via crossdisciplinary research activities, (b) port data-management and scientific workflow codes to the regional computational resources and optimize to the regional connectivity bandwidth limitations, and (c) implement and deploy visualization software for developing collaborative virtual spaces.
- **Objective 7:** Optimize scalability of existing climate codes and develop new climate codes for the infrastructure provided by the project.
- **Objective 8:** Exploit the benefits of visualization in cultural heritage research: (a) prototype a small, portable imaging center at CaSToRC, and (b) produce software tools for tele-immersive collaborative environments.
- **Objective 9:** Develop an online cultural heritage digital library for the Eastern Mediterranean.
- **Objective 10:** Port existing common and new algorithms at synchrotrons to GPUs.

Some of LinkSCEEM’s accomplishments are briefly outlined below.

**COMPUTATIONAL ECOSYSTEM FOR THE EASTERN MEDITERRANEAN**

LinkSCEEM successfully developed an operational model for an integrated HPC e-Infrastructure. Two regional HPC facilities have contributed resources and services in this project. The Cyprus Institute (CyI) through CaSToRC contributed Cy-Tera, an HPC facility of 35 Tflops peak performance, with an associated research and educational program devoted to computational science.

The BA installed a Sun cluster of peak performance of 11.8 Tflop/s, and also maintained an archival system. BA had storage systems of 3.7 Pb, of which 1.6 Pb were previously unused. The BA was engaged in joint activities and partnerships in visualization projects with universities in
Egypt, the region, and internationally. The consortium subsequently administered this e-Infrastructure and various access calls for regional computational scientists.

Access to the systems was given through frequent calls for proposals. Users could apply for three types of access:

- **Production.** A large number of computational resources were granted over a 12-month access period for scientific computing.
- **Preparatory.** A small amount of resources were allocated over a 6-month period for code development and testing.
- **Educational.** Resources were allocated for educational purposes (for example, to lecturers and students of university courses).

The access calls for preparatory and educational access were continuously open. Production access calls were issued twice yearly.

Figure 1 identifies the scientific field and principal investigator home country for the computational projects carried out on the infrastructure.

Figure 1. Scientific fields and countries represented in the computational projects carried out as part of LinkSCEEM’s integrated HPC e-Infrastructure.

All applications underwent a rigorous and transparent review process, which ensured that the expensive computational resources were put to good use. Preparatory and educational access requests only underwent a brief technical review to ensure that the proposed applications were suitable for the available systems. These requests were usually processed within a few days. Production access applications underwent a more elaborate process as the allocated computer time was significantly larger. These applications underwent a peer-review process of international standard, which ensured the fair and transparent allocation of resources to users based on scientific excellence. The process included a technical review and a scientific assessment by international experts. It is a significant success of LinkSCEEM to have been consistently able to identify and motivate international experts to scientifically review proposals submitted by regional scientists. A total of 87 production projects and 183 preparatory access projects were accommodated on the supercomputers, resulting in 76 scientific publications from 53 completed projects and more than 80 presentations in conferences and scientific meetings.
One of the success stories of LinkSCEEM has been the availability of a training cluster to the Eastern Mediterranean region. This cluster, called Euclid, was hosted at the CyI and was a hybrid CPU/GPU Linux cluster composed of six 8-core computer nodes with two NVIDIA Tesla T10 processors attached to each node. Academic institutions were given access for teaching purposes. Euclid was also used for training events and user meetings, where trainee user accounts could be set up for hands-on training. Individual users who were starting with parallel programming and required a cluster for their educational and testing needs were also given access.

REGIONAL TRAINING PROGRAM

LinkSCEEM implemented an ambitious training workshop program. The program consisted of an annual series of five large 3-day workshops that were held in alternating locations across the Eastern Mediterranean. The program included one large cross-sectional workshop (usually in winter) and a General User meeting (usually in the summer) on general HPC-related topics such as parallel programming, performance analysis, and HPC applications. This was supplemented with three workshops in the project thematic areas (climate modeling, cultural heritage, and synchrotron radiation). The thematic workshops focused on community-specific lectures regarding methods and applications. In total, the project organized 20 workshops as part of this training program.

Complementing the intensive multiday workshop program was a series of relatively brief basic training sessions cast into the format of an HPC roadshow. The aim of this event series was to promote the available HPC facilities and provide basic training in how to access and use the supercomputers. In addition, very detailed presentations were given regarding available training events in general and online training materials in particular. All participants were offered access to Euclid, the LinkSCEEM training system and connected during the event, when possible. This was a very effective way of tempting new users into a supercomputing environment. The format of the roadshow was designed to maximize impact and outreach while minimizing organizational overhead. All roadshow events followed a predefined program that was also made available in video and audio. This meant that local trainers could be relatively easily recruited and many events were organized locally without having to pay for relatively expensive regional travel. The format of the roadshow proved very successful. More than 800 people participated in 37 single events in the framework of 3 integrated roadshows.

Figure 2 shows the number of LinkSCEEM events carried out throughout the region.
One major highlight of the LinkSCEEM project was the organization of the Conference on Scientific Computing (CSC 2013), which took place in Cyprus in December 2013. Leading international researchers in computational science gathered to present highlights of their scientific work performed using Partnership for Advanced Computing in Europe (PRACE) and LinkSCEEM computational resources (see Figure 3).

CSC 2013 brought together 120 international computational scientists, amongst them the directors of the largest HPC facilities in Europe and the US. The European research community, local academics, and scientists from the Eastern Mediterranean region and US had the opportunity to exchange ideas, develop synergies, and set out a vision for future development on various aspects of HPC.

LinkSCEEM also had other dissemination activities. In principle, three dissemination channels were used to actively promote the project. The first channel was the events organized by the project, the second was the participation in regional and international conferences and meetings, and the third was the project website. In addition, the project was also acknowledged in the publications of users. In total, LinkSCEEM was presented in 109 dissemination activities.

Figure 3. Professor Bothina A. Hamad from the University of Jordan at the 2013 Conference on Scientific Computing. She was assisted through LinkSCEEM to install the first cluster enabling research in computational solid state, projects, and access to Cy-Tera.

MIDDLE EASTERN WOMEN IN SCIENCE PROGRAM

LinkSCEEM also ran a Middle Eastern Women in Science program, which supported women in various ways as they engaged with computational science. As an example, a European contribution through the LinkSCEEM project provided funding for fellow Hadeer EL-Habshy (see Figure 4) to attend a workshop program at the Jülich Supercomputing Centre in Germany.

RESEARCH ACTIVITIES

LinkSCEEM’s crossdisciplinary activities are aimed at research on simulation techniques across scientific fields, and at providing sophisticated support in the optimization of algorithms used in HPC applications. The crossdisciplinary research team worked in close coordination with the user support group and also significantly contributed to training activities. Their approach toward performance analysis and optimization was based on existing efforts and experiences.
within the Virtual Institute for High Productivity Supercomputing (VI-HPS). A number of tools were installed on all systems to target specific aspects of performance, such as single-node performance, parallel performance, debugging, instrumentation, measurement, and visualization. Training events showcasing some of these tools were provided throughout the project.

Climate Modeling Research

LinkSCEEM’s climate modeling research successfully brought expertise to and subsequently enabled research at the forefront of climate studies of the Eastern Mediterranean region. The parallel scalability of the atmospheric general circulation model that is used to predict regional climate change was improved as part of the research done in LinkSCEEM.

Cultural Heritage Research

The objectives of LinkSCEEM’s cultural heritage research were twofold. The first task was to establish a novel small-object imaging center at CaSToRC that would make use of multiple high-resolution imaging techniques for the documentation of a wide range of ancient artefacts. The center was designed to focus in particular on two innovative approaches to imaging: reflectance transformation imaging and 360-degree imaging of cylindrical objects, especially cylinder seals. A second goal was to collaborate with the InscriptiFact Digital Image Library to facilitate the worldwide distribution of the center’s images. This objective was broadened throughout the project duration as it became possible to extend InscriptiFact capabilities by developing a tailor-made content management system that was tuned for regional artifacts by the use of the open source MEDICI software. InscriptiFact is designed to host a very limited number of digital formats, mainly linked to inscriptions. MEDICI however, allows hosting of a wide range of digital formats, including 3D models.

In addition, a tele-immersive visualization system that would create a portable, virtual collaborative space where scholars could jointly examine artefacts in a 3D environment was developed and tested across the region.

Figure 4. Fellow Hadeer EL-Habashy (middle row, far right): “When I got accepted to the Guest Student Program on Scientific Computing, Jülich Supercomputing Centre (JSC), Germany, I realized that it marked a turning point in my career.” EL-Habashy received support to attend JSC as part of LinkSCEEM’s Middle Eastern Women in Science program.
Synchrotron Radiation

Synchrotron radiation facilities such as the Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) and the European Synchrotron Radiation Facility (ESRF) enable scientific research in a broad variety of fields: atomic and molecular physics, biology, material science, spectroscopy, archaeology, and imaging. LinkSCEEM contributed significantly to the efforts to support SESAME in developing the ecosystem around the emerging synchrotron, which became operational in 2016. The research conducted under LinkSCEEM sought to

- port existing synchrotron applications to GPUs,
- develop new synchrotron applications for GPUs, and
- support training programs for future SESAME users.

The research was conducted by experienced researchers at the ESRF jointly with staff at SESAME. Many exchanges and visits ensured that the generated knowledge was also transferred to SESAME so that development could continue on the ground beyond the duration of LinkSCEEM. The research on synchrotron applications mainly focused on the use of accelerators, in particular graphic processing units (GPU), in synchrotron data processing within LinkSCEEM.

Beyond the provision of computing resources and training to computational scientists, LinkSCEEM also developed data-management systems for regional use and provided performance analysis tools and expertise for application support.

The project conducted research in three thematic areas of high regional relevance. The consortium contributed to developments by porting and accelerating HPC applications in the fields of climate modeling and synchrotron data analysis. Furthermore, an advanced imaging facility for cultural heritage applications was installed and operated by the project. Examples of the science enabled by LinkSCEEM are shown in Figure 5.

Figure 5. Examples of the science enabled by LinkSCEEM. (a) Modeling of supernovae explosions. (b) Modeling of aquatic swimming robot tentacles for the development of bioinspired robotic devices. (c) Modeling of layered materials (such as graphene). (d) Probing new physics beyond the standard model. (e) Modelling proteins to enhance the understanding of cancer development.
CONCLUSION

LinkSCEEM has had a strong impact on the scientific communities of the wider region. Significant computational resources were available across the region through a transparent excellence-based allocation process for the first time. This introduced regional scientists to international best practice and increased the competitiveness on a global level. Thanks to LinkSCEEM, a number of scientists were able to scale up their research work to fully use the opportunities of computational science similar to their counterparts in central Europe and the US. Furthermore, by being familiar with the access mechanisms introduced by LinkSCEEM, regional scientists will find it easier to compete for access to very large systems, as provided through PRACE. The impact of these scientists spreading their know-how to colleagues and local institutions should be emphasized, because this is an important instrument in establishing an HPC tradition.

The provision of computational resources to computational scientists has had a direct, profound scientific impact—this is apparent by the number and quality of the publications resulting from the scientific work done on the supercomputers available through LinkSCEEM.

Given that, at the end of LinkSCEEM, it was apparent that the regional scientific community required access to supercomputing systems to carry on, The CyI’s and BA’s provision of computational resources has continued. As of September 2017, two and a half years after LinkSCEEM ended, regional preparatory applications were still being received and applications were being accepted for the 12th Call for Production.

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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\textsuperscript{1–3} founded on the fundamental sciences\textsuperscript{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.
with sizes ranging from a few to several tens of atoms/molecules. In the past, learners had to contend with 2D static structures on textbooks 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. 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.

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. 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. 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.

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.
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) 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. 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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Making Supercomputing Available to All Cuban Researchers

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Scientists in Cuba must get up to date with the latest trends and best practices in scientific computing. As a consequence of the socioeconomic and geopolitical situation in and around Cuba, a lack of financial means restricts Cuban researchers’ access to the supercomputing infrastructures, techniques, and tools that are urgently needed to support the increasing use of computational tools and efficient data processing in different areas, especially those related to public health.

In the following article, I recount my story as a young researcher and my efforts to make nationwide high-performance computing (HPC) services available to all Cuban scientists. This effort was motivated by my research experiences 15 years earlier. I began working with complex images acquired with a low signal-to-noise ratio (SNR), and found myself faced with the problem of phase residues, a major drawback for the bidimensional phase unwrapping process that is usually performed when processing phase images in several health-related applications. My experiments applied de-noising algorithms to complex images combining nonlinear filters based on order statistics methods in the wavelet domain, which demanded high computational power. The unavailability of HPC facilities imposed severe challenges for the research process required to achieve my proposed objectives.

DE-NOISING COMPLEX IMAGES

I graduated in 1999 from the School of Electrical Engineering of the Universidad Central “Marta Abreu” of Las Villas (UCLV) in Cuba. Since 2003, I have been linked to the Center for Studies on Electronics and Information Technologies (CEETI), where I did my PhD studies on de-noising complex images, meanwhile I served as head of the Telecommunications Department in the Electrical Engineering School. Upon receiving my PhD in 2007, I was nominated to and accepted the role of director of the UCLV Central ICT Department.
My research involved formulating and testing a set of algorithms using simulated, phantom, and real images, which showed improvements in the SNR (see Figure 1) and image quality (see Figure 2) when using combined methods (nonlinear ordering statistics and wavelet domain algorithms such as NLSUFD1AD, and NLSUFD1AD).

To work with raw real data, the phantom images used during the research were obtained with an experimental tomograph installed at the Centro de Biofísica Médica (Medical Biophysical Center) in Santiago de Cuba. Those images had to be processed in Santa Clara, 650 km away, on a small cluster of 12 power desktop computers.

The usage of nonlinear ordering statistics methods implies an extra computational burden inherent in calculating angular distances. The simulations started to delay more than a week with the available hardware, making experiments nonviable. Additionally, the electrical supply suffered shortages and the lack of electrical backups and limited air conditioning systems in conjunction with the low-quality hardware available imposed extreme conditions on my research.

Finding a solution in Cuba to shorten the time of the experiments and progress more rapidly in my research was not possible, because there were no available super computation infrastructures in the country. Many experiments had to be performed remotely in HPC clusters in Canada, Spain, and Belgium through narrow bandwidth links. In 2007, UCLV had an Internet connection of 1 Mbps, shared across all university services. This link was congested during the day, so early morning (from 1 AM to 6 AM) became the ideal time for experimentation.

Despite the passing of time and technological advances, the situation continues to repeat itself. Investigators at important research centers in Cuba, such as the Centro de Neurociencias de Cuba (Cuban Neuroscience Center, or CNEURO), have a 3-T magnetic resonance tomograph that allows them to obtain functional magnetic resonance imaging (fMRI) to follow up on drug treatments of cancer-related brain lesions, among other applications. The lack of sufficient supercomputing capabilities to process this data within tolerable times means that the researchers must send high-resolution images to Canada to be processed—and deal with the storage limitations and Internet congestion that still confront Cuba.

Since 2007, I have led international collaboration projects related to ICT infrastructure. From 2013 to date, I have coordinated the Cuban side of the ICT-NETWORK program between Flemish universities in Belgium and five Cuban universities. Within this collaboration’s framework, I have explored opportunities to strengthen computational research capacities for Cuban scientists.

Figure 1. Algorithms with better performance SNR for gradual increments of noise ($\sigma$) over the phase images shown in Figure 2.
BIRTH OF THE HPC-CUBA PROJECT

Researchers rely more and more on scientific computing. In their efforts to transform research data into knowledge, Cuban researchers are restrained by their limited knowledge of and access to technologies and tools for efficient data processing. These limitations can be alleviated by providing expertise and access to scientific computing infrastructures for researchers from a wide range of institutions, which would in turn provide opportunities for synergy and application license sharing. It was discovered that difficulties arise mainly in the following aspects: access, autonomous management of research applications, data science knowledge, and effective coding for parallel/distributed processing.

The idea of making supercomputing available to all Cuban scientists was born in 2015 when I met Dieter Roefs in Belgium (Datacenter Coordinator of Ghent University), starting with two small HPC clusters installed in Santa Clara (UCLV) and Santiago de Cuba (UO). Thanks to big donations from Ghent University in Belgium (besides VLIR-UOS funded purchases), various supercomputer clusters were shipped to Cuba. Two IBM clusters were installed in Havana (UCI) and Santa Clara (UCLV), with 84 nodes, 600 cores, and 2 Tbytes of RAM each. Two GPU Nvidia K80 cards were also installed in Santa Clara. Similar capacities with Dell technology were installed in Santiago de Cuba (UO). This signaled the start of the HPC-Cuba project (see Figure 3).

Although this infrastructure is available at some universities, it is not accessible to all potential users from surrounding research groups and scientific institutes. Nationwide access will remain problematic as long as there is no established national center for scientific computing to provide a broad user base of researchers with a platform and portal to access to HPC and big data services. The HPC-Cuba project has a geographic distribution of HPC infrastructure at three points, the strongest Cuban universities in terms of ICT infrastructure: UCI in Havana (west), UCLV in Santa Clara (central), and UO in Santiago de Cuba (east). Several free software-management platforms have been installed for services orchestration (foreman), configuration management (Puppet/Ansible), and management of computing resources (slurm) with CentOS, as well as a national Lightweight Directory Access Protocol (LDAP) system for access to distributed infrastructure.
Technology and knowledge transfer are attracting industry (for example, BioCubaFarma) to merge their computational infrastructures with the proposed network. Industry and its associated research centers play a key role in the sustainability of the project. We have identified a group of enterprises and associated research centers producing cutting-edge technology products (CNEURO, FINLAY, CIM, CIGB, all of them belonging to BioCubaFarma). ETI-BioCubaFarma, a hub that provides supercomputing services to the most important research centers in Havana (Biocubafarma consortium), will acquire a supercomputing infrastructure and share it through the HPC-Cuba project. Other centers and research laboratories in the country, especially those associated with in silico experimental modeling, are already benefiting from this initiative, for example, Centro de Bioactivos Químicos (Chemical Bioactive Center) at UCLV and Laboratorio de Química Comutacional y Teórica (Computational Chemistry Lab at Havana University). So Cuban scientists are now closer to accessing a national center for scientific computing (see Figure 4).
As scientists are often not IT experts, they face difficulties managing the applications they require; there is a need to adopt solutions to ease deployment and configuration of applications. UCLV HPC staff adopted EasyBuild, which is based on open source project. We have even submitted contributions to the EasyBuild community.10

There is no lack of challenges to face, as researchers are often dealing with difficulties when analyzing large amounts of heterogeneous and dynamic data (for example, big data and deep learning). There is a need to provide users with techniques for intelligent data analysis and code optimization for parallel applications. This would allow them to effectively use the available compute capacity—rather than depending only on generic analysis techniques and single-node computations—and thus convert their data into highly valuable knowledge.

CONCLUSIONS

The HPC-Cuba project initiative enables, supports, guides, and trains Cuban researchers to maximize their scientific output based on scientific computing services. In this way, we are influencing the quality and quantity of research conducted at various institutions at the national level, thus contributing to the general sphere of interest—science contributing to national development.

ACKNOWLEDGMENTS

I would like to thank the University of Ghent (Ugent) for its donation of HPC infrastructure, and VLIR-UOS for its support through international collaboration projects; Dieter Rose, datacenter coordinator at Ugent, as one of the founders of the HPC-Cuba project; Prof. Dr. Dirk Rose, KU Leuven, for supporting this project idea; Prof. Dr. Esteban Moëskos, Universidad de Buenos Aires, for opening a door to the regional HPC community; and Kenneth Hoste and Ugent HPC staff, VSC/ Flemish Supercomputer Centre, and Dr. Damian Alva-rez, Jülich Supercomputing Centre, for training our HPC staff and all the support offered. Special thanks to the Cuban HPC staff for all of their valuable efforts.

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Doing Research under Extreme Conditions

Amir Hossein Darooneh
University of Zanjan

Despite drastic cuts to university and research institute budgets, research activities by Iranian scientists has continued. This article presents work being performed by the Complex System Group at the University of Zanjan. Most of the computational works are carried out on multicore processors or parallelized manually on different PCs.

Knowledge promotion is one of the simplest and most direct ways to improve life in all its dimensions. The main responsibility for such promotion lies with scientists. There is no difference between scientists around the world—together they form a unique body, without consideration for geographic region. Any deletion or omission would damage this body and, consequently, have an unfavorable impact on the ideal picture of a peaceful world. As scientists, our mission is to protect world peace and human dignity. Therefore, we should keep our integrity and eliminate obstacles to scientific research.

In the following article, I describe the difficult research conditions in Iran, including being deprived of access to needed facilities, particularly for high-performance computing (HPC). I also explain our efforts to overcome these difficulties.

THE COMPLEX SYSTEMS GROUP AT THE UNIVERSITY OF ZANJAN

The University of Zanjan is a public university located in Zanjan, the capital of the Zanjan province and one of the largest cities in the Iranian Azerbaijan region. It is situated 298 km northwest of Iran’s capital, Tehran.

Founded in 1975, the University of Zanjan is one of the largest universities in the country. It has four faculties—engineering, sciences, humanities, andagricultures—and hosts a community of approximately 400 faculty members and more than 10,000 students.

The University of Zanjan’s Department of Physics was established in 1989 as a part of the Faculty of Sciences. Nowadays, the department includes 27 faculty members working on the major fields of condensed matter physics, nanophysics, complex systems, atomic-molecular physics, and astrophysics.
The University’s Complex Systems Group (CSG), which I head, began in 2006 by taking master’s and doctoral students. In CSG, we investigate the statistical and dynamical properties of various complex systems to understand the governing rules of their behaviors and the underlying physics. Currently, CSG includes one faculty member, five PhD graduates, and six PhD students (see Figure 1). We also collaborate with researchers and faculties at other universities, whether in Iran or abroad.

![Figure 1. Members of the Complex Systems Group, in front of the University of Zanjan’s Faculty of Sciences (April 2010).](image)

**COMPLEX SYSTEMS GROUP ACTIVITIES**

Here, I briefly describe the projects that have been accomplished by or are currently underway in our group.

**Structural Properties of Real Complex Networks**

Most of our research in this area focuses on the properties of earthquake networks. Our aim is to find connections among the topological properties of earthquake networks and the empirical laws of seismicity. We are also interested in research on earthquake forecasting.\(^1\)\(^-\)\(^5\)

**Dynamical Processes on Complex Networks**

Our main object here is studying how the dynamics of a process are affected by the mesoscopic structural properties of networks. The existence of chimera-like states in the synchronization process, suppression of explosive synchronization, and changes in the spreading rate of diseases are just a few of the consequences of the mesoscopic structure of networks.\(^5\)\(^,\)\(^7\)

Environmental randomness also influences the dynamics of a process. For example, in the voting process, the rate of consensus changes when some nodes with constant opinion (zealots) exist. The fixation probability and fixation time are significantly altered in the evolutionary dynamics if we consider random distribution for wild-type or mutant fitness (see Figure 2).\(^8\)\(^-\)\(^10\)

**Natural Language Complexity**

Text can be considered a complex system: words are its constituents that interact with one another through grammatical rules and meanings. The concept of a text is the collective behavior of the words within it. We are interested in studying the properties of text by using methods such as fractal pattern analysis, complex network theory, and nonextensive statistical mechanics. The results are used for text-mining issues and genomic and proteomic data analysis.\(^11\)\(^-\)\(^17\)
Fractal Structures in Complex Fluids

In this area, our goal is the experimental and theoretical study of complex fluids. Fractal structures in fluids is the main theme of our research. In particular, we are interested in studying the spread of surfactants and their instabilities on fluid layers.\(^{18}\) We intensively use image processing algorithms to find the fractal dimension of the observed structures in our works.

Time-Series Analysis

We are taking two approaches to time-series analysis. First, we are interested in unifying and finding the relation among different methods for measuring complexity in systems. Second, we are analyzing complexity in real systems. Quantifying climate change, classifying climate, and diagnosing brain (psychological) diseases from associated series are also topics of interest.\(^{19-22}\)

TRAINING FOR HIGH-PERFORMANCE COMPUTING

The students in our department are taught HPC through short (one-day) unofficial courses. They are acquainted with the concept of parallel programming, multicore processing, CPU cluster computing, and the parallel algorithms on GPU. Unfortunately, we are faced with a lack of facilities to provide HPC. Although a few private companies and public institutions provide HPC services, they are more expensive and university funding cannot cover the cost of using them. International services are beyond our reach. For a long time, our requests to download open source software were rejected by sites such as Sourceforge, Nvidia, and Google Code. Many Iranian scientists have unofficially used HPC services in foreign institutes and universities with the help of their colleagues in other countries. I personally had the opportunity to use a cluster with 192-nodes during sabbatical leave at the University of Waterloo in Canada.

The CSG office in the Faculty of Sciences building, where our group members perform their studies, is equipped with multicore PCs. They are used for simulations and calculations with OpenMPI and Openmp but can hardly meet our research demands. We had access to 64-node cluster processors but it is down due to maintenance difficulties (buying spare parts) and university budget cuts. Hence, we face difficulties with numerical and simulation works. We are trying to get financial support from the Ministry of Science, Research and Technology, but this is a bureaucratic, time-consuming process.
Moreover, restrictions on international money transfer cause many problems for us. For instance, this issue has affected payment of fees for publication of our reports or participation in scientific events.

CONCLUSIONS

As a final point, on behalf of CSG, I would like to express appreciation for our colleagues around the world for their spiritual and material support. This is what makes our world a better place in which to live. We also thank Nature Springer and the Public Library of Science for helping us by waiving publication fees. Our special thanks goes to the editors of Computing in Science & Engineering for publishing this article.

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A new generation of computational scientists is currently being trained across Costa Rica, mainly at research laboratories in public universities. This new wave of scientists is expected to further increase the impact of advanced computing in conceiving creative, powerful ways to understand the universe and solve complex problems.

Since its creation in 1999, the Costa Rica National High Technology Center (CeNAT; http://www.cenat.ac.cr/en/) has fulfilled a fundamental role in fostering interaction among the triple helix—academia, government and industry—through the use and development of high-technology products and services. The Advanced Computing Laboratory belongs to CeNAT. Our laboratory’s philosophy is that advanced computing catalyzes scientific discovery and technological innovation. We truly believe algorithms, data structures, and computer architectures have a transformative power to bring about groundbreaking solutions to the most pressing problems in science and engineering.

I am a computer scientist by training and an expert in high-performance computing (HPC). My research concentrates on parallel programming models and fault-tolerance strategies for HPC systems. Yet, my interests extend to all aspects of advanced computing: modeling, simulation, and massive data processing (see http://www.emeneses.org/ for a good collection of my research work).

I began my research career as an instructor in the School of Computing at the Costa Rica Institute of Technology (ITCR) in 2001. I still hold a partial appointment at ITCR as an associate professor of graduate studies. I obtained a PhD in computer science from the University of Illinois at Urbana-Champaign in 2013. After graduation, I was hired as an assistant research professor in the Center for Simulation and Modelling (SaM) of the University of Pittsburgh. In 2015, I

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returned to Costa Rica and resumed my academic career as a professor at ITCR. A year later, I took over responsibility as director of the Advanced Computing Laboratory at CeNAT.

Leading the Advanced Computing Laboratory at CeNAT has been an exciting experience. Not a week has passed without finding new colleagues, collaborations, funding opportunities for high-potential projects, or promising research ideas. The CeNAT is in a strategic position since it is part of (and funded by) the national system of public universities. This means that we have a direct connection to scientists and engineers with concrete needs in terms of how to accelerate their simulations or data processing tasks. Our lab at CeNAT employs approximately 15 people, half of them permanent staff, the other half student assistants (see Figure 1). Our members have either electrical engineering or computer science backgrounds. All staff have solid computer programming skills that they use to enrich science with computational tools through a side-to-side collaboration with the scientists and engineers who utilize those tools. We maintain our own computer cluster, participate in research projects, write papers, look for funding opportunities, teach workshops (R, Python, MPI, OpenMP, and OpenACC), and organize academic events. We also very much enjoy working with colleagues from areas as diverse as biology and political science. To learn more about our research projects and services, you can check out our webpage (http://cluster.cenat.ac.cr/).

As far as I know, our lab is the only unit in Costa Rica’s academic environment devoted to the research and development of advanced computing. However, there are several other laboratories and centers working with computational science and engineering tools. Some of them also own computer clusters. In fact, we have identified more than 20 such computer clusters in the country. Those infrastructures belong mainly to academic units in physics departments across the national system of public universities. There are a few efforts on the government side as well. As for industry, we maintain contact with a couple of groups.

One key goal in our lab is to grow the community of users of our advanced computing services. We organize an annual High-Performance Computing School to train people on HPC programming languages and tools. Approximately 50 people attended the most recent event. In addition, we lead the Scientific Computing Research Network (RICC), which serves as a platform to interact with people interested in advanced computing tools and services. The RICC organizes workshops, talks, and a scholarship program to build bridges among scientific domains. Thanks to these initiatives, our user base is growing stronger.

There are three domains that stand out for burning cycles on our computer infrastructure: oceanography, machine learning, and bioinformatics. Computational oceanography helps in predicting...
waves on both coasts of the country. Machine learning is used to tackle signal processing challenges, including those associated with cancer research. Bioinformatics is mostly used to assemble and analyze genomic sequences from a wide range of species (from viruses to trees). Other domains represented in our user base are computational seismology, physics simulations, computational bioacoustics, image analysis, big data processing, and computational neuroscience. Figure 2 presents a visualization of a quake on a volcano in Costa Rica that was created by our collaborator Yuen Law-Wan from RWTH Aachen University. This is just one example of the type of projects being carried out using our advanced computing tools and services.

![Figure 2. Visualization of seismic activity on a volcano in Costa Rica created by CeNAT collaborator Yuen Law-Wan of RWTH Aachen University.](image)

Other initiatives complement our efforts in promoting the use and development of advanced computing. Master’s and doctorate programs provide a platform to develop theses on computational science. Courses on simulation, parallel computing, and computational science are regularly offered as part of those programs, providing a venue for training in the area. There is, however, no specific computational science program in any university in Costa Rica.

A new generation of computational scientists is currently being trained at several institutions across the country, including the Advanced Computing Laboratory at CeNAT, some research laboratories at the University of Costa Rica, the eScience program at the Costa Rica Institute of Technology, and others. We expect this new wave of scientists will further increase the impact of advanced computing in conceiving creative and powerful ways to understand the universe, and solve complex problems.

**ABOUT THE AUTHOR**

Esteban Meneses is director of the Advanced Computing Laboratory at the Costa Rica National High Technology Center (CeNAT). His research interests include resilience techniques for HPC systems and parallel programming models. Meneses received a PhD in computer science from the University of Illinois at Urbana-Champaign. Contact him at esteban.meneses@acm.org.
Although computing research and facilities in Latin America have been developing steadily, a remarkable gap nevertheless remains in the availability of resources and specialized human resources compared to other regions. RICAP (Red Iberoamericana de Computación de Altas Prestaciones, or Ibero-American Network for High-Performance Computing) aims to fill this gap by means of a strategic and advanced computational infrastructure that includes both high-performance and high-throughput computing platforms. This network will also develop software tools to facilitate this infrastructure’s accessibility and computational efficiency to encourage use by the Latin American computing community as well as focus on strengthening and training human resources in both parallel programming techniques and large-scale computing platform operations.
Red Iberoamerica de Computación de Altas Prestaciones (Ibero-American Network for High-Performance Computing)—known as RICAP—is a new consortium that was created to provide Latin America with advanced ICT services. In particular, a strategic cloud-based infrastructure based on advanced architecture for scientific computing has been developed that includes both high-performance computing (HPC) and high-throughput computing (HTC).

RICAP—which is funded by the Ibero-American Programme on Science and Technology for Development, known as CYTED—began on 1 January 2017 and will run until at least 31 December 2020. At the kick-off meeting, RICAP included:

- eight Latin American computing centers: CSC-CONICET (Argentina); UFRGS (Brazil); SC3-UIS (Colombia); UCR (Costa Rica); CIEMAT (Spain), BSC-CNS (Spain); and CUDI and CINVESTAV (Mexico);
- one of the world’s largest supercomputing vendors (Fujitsu); and
- an experimental Latin American consortium in the field of physics (LAGO).

Three additional institutions joined the consortium in 2017: Uniandes (Colombia), CEDIA (Ecuador), and the National Supercomputing Center/Universidad de la República (Uruguay).

This network aims to boost the development of different tools to ease access and improve computational efficiency of HPC infrastructure. Another key objective is to encourage infrastructure use through dissemination and outreach actions that are expected to attract users from various universities and other scientific and industrial areas. RICAP is supported by RedCLARA, which develops and operates the only Latin American advanced Internet network, and by SCALAC, an advanced computing consortium to extend services throughout Latin America and the Caribbean. RICAP is strongly promoting the integration of new nodes (partners) in the Ibero-American countries that were not initially attached to it, as demonstrated by its integration of Uniandes, CEDIA, National Supercomputing Center, and Universidad de la República.
The project seeks to make HPC resources more readily available to the community, thereby providing a real alternative to proprietary services located outside the region. Specific objectives include the following:

- effective interconnection of high-performance open services from the clusters provided by RICAP (both supercomputing and cloud access);
- implementation and subsequent promotion of solutions for the access and operation of this software-based network;
- design and development of open-source tools that improve the computational efficiency of the infrastructure (especially in an environment such as the cloud) in an unattended and dynamic way;
- promotion and transfer of knowledge of RICAP solutions and services by way of courses and seminars for administrators and end users on the latest technologies in HPC and HTC; and
- collaboration with other national and regional initiatives (RedCLARA, H2020, and others to be identified).

Achieving these objectives will allow different Latin American groups—for whom it was previously extremely difficult to perform large-scale research on either data analysis or simulation because of the lack of sufficient computing power—to carry out new activities. These groups will also be able to collaborate with Spanish research centers such as CIEMAT or BSC-CNS as well as with leading Latin American groups belonging to RICAP. In this sense, RICAP brings value to the scientific and technological community in several of its fundamental dimensions: infrastructure and software development; value-added services for advanced academic networks; and ICT solutions that support research.

ANTECEDENTS

RICAP is a recent collaborative network based on the efforts of other previous and present initiatives. As the first seeds, the work by RedCLARA and the HTC projects articulated around it (for example, the EELA series, CHAIN series, and MAGIC) should be mentioned. The Panamerican Association of National Research and Education Networks has provided not only connectivity to the academia, but direct support to research communities, specific calls to access to infrastructure, and many other activities that have promoted computer and computational sciences in Central and South America.

Some years ago, an FP7 (7th Framework Programme for Research and Technological Development) collaboration project called Red Iberoamericana de Supercomputación (RISC) was established as a network to support the coordination of supercomputing research between the EU and Latin America. It aimed to deepen strategic R&D cooperation between the two regions in the field of HPC by building a multinational and multistakeholder community that involved significant representation of relevant researchers, policy makers, and users. RISC worked to identify common needs, research issues, and opportunities in the transition to multicore architectures across the computing spectrum and relevant programming paradigms, algorithms, and modeling approaches, thus setting the basis for the formulation of a global strategy for future research.

Another very important initiative that is still on the way is the Servicio de Cómputo Avanzado para Latinoamérica y el Caribe (Advanced Computing Services for Latin America and the Caribbean), or SCALAC. Similar to RICAP, SCALAC is a consortium of centers in several Latin American countries dedicated to the development of HPC and scientific computing in Latin America. These centers have been organized, with the support of RedCLARA, to jointly and collaboratively provide advanced computing services in the region. SCALAC members are centers that have advanced computing resources, belong to universities and scientific research institutions, and are supported by the advanced research and education networks of their countries. The formal launch of the SCALAC community was on 1 March 2013 at the Universidad Industrial de Santander in Bucaramanga, Colombia.
Jointly with these projects, there is an effort in the region to promote HPC through international conferences that unite researchers to present their activities and latest developments. Such networking activities are the seeds of future collaborations. In the HPC field, two major conferences were organized in Latin America up to 2014: CLCAR and HPCLATAM. In 2014, these two conferences merged into a single major event that gathers the entire HPC/distributed computing research community: the Latin America High Performance Computing Conference (CARLA). The most recent CARLA was held in Buenos Aires in September 2017, with more than 100 participants from more than 25 countries representing America, Europe, Asia, and Oceania. It is also worth mentioning the recent organization of a flagship conference on cluster, grid, and cloud services—the 16th Annual IEEE/ACM International Symposium on Cluster, Cloud, and Grid Computing—held in 2016 in Cartagena, Colombia.

Another important topic in any scientific discipline is training, which will be discussed later in this article.

PLANS TO PROVIDE REAL ADDED VALUE TO THE IBERO-AMERICAN COMMUNITY

This section provides information about the infrastructure being made available for free by RICAP and the methodology for accessing it.

Accessing RICAP Resources

The proposed methodology is similar to that followed by large computing infrastructures such as PRACE in HPC or FedCloud in HTC, in which different nodes hosting computing clusters and computing capacities are federated. However, in RICAP, this federation will be kept as simple as possible to facilitate easy access and administration.

Access to the strategic infrastructure of RICAP will be carried out in two ways. First, there will be online open calls for proposals for the use of supercomputers from which CPU and/or accelerator hours (GPU and Xeon Phi) will be granted by a committee designated by RICAP. In this call, storage and transfer capacities of data will also be granted to the final user (from any Ibero-American country, not only those that have a partner within RICAP). Second, RICAP will enable a cloud infrastructure especially suitable for HTC. It will be accessible via either command line or a user-friendly web interface. The availability of the cloud infrastructure will be continuous and uninterrupted.

This scenario requires open-source solutions that improve computational efficiency in heterogeneous and dynamic environments. Therefore, RICAP will develop and provide tools that maximize this computational efficiency beyond what has already been successfully put into production.

In relation to the HPC environment, fault-tolerant developments that will equally improve the use of supercomputers will also be used and have been conveniently tested by the RICAP groups. These solutions are based on managers and tools mostly used in the Top500, such as resource managers, checkpoint and load-balancing libraries, and message-passing libraries. They will be transparent to the end user and exploitable by administrators. An exploratory work can be found in “A Simple Model to Exploit Reliable Algorithms in Cloud Federations.”

All of these developments will converge into tools that combine dynamic checkpointing and fault-tolerance capabilities with cloud job resource managers over CPU and accelerators. Container management in virtualized HPC environments will also be studied.

Work in HPC environments and the cloud will produce user statistics and usage modes, as well as a measurement of computation times, tools used, and success stories. This information will be useful not only in the design and development of future administrative applications, but also in the improvement of existing ones in each RICAP center.
Infrastructure

Table 1 describes the strategic HPC infrastructure of RICAP, which is connected internally by Infiniband and externally with fiber optics by the corresponding academic networks associated with RedCLARA.

Table 1. RICAP’s HPC infrastructure.

<table>
<thead>
<tr>
<th>Academic network</th>
<th>Country</th>
<th>Description of cluster</th>
</tr>
</thead>
<tbody>
<tr>
<td>BSC</td>
<td>Spain</td>
<td>General-purpose cluster with 165,488 Intel Platinum cores in 3,456 nodes, with more than 394 Tbytes of main memory and 25 Pbytes of storage</td>
</tr>
<tr>
<td>CIEMAT</td>
<td>Spain</td>
<td>One cluster with 680 Intel Gold processors and 456 cores Xeon Phi, one cluster of ~100,000 Nvidia cores, two cloud nodes with ~950 cores CPU, and more than 1 Pbyte of storage</td>
</tr>
<tr>
<td>CEDIA</td>
<td>Ecuador</td>
<td>12 computing nodes with 322 Intel Xeon cores, 1 Tbyte RAM, 6 Tbytes of storage, and 5,760 Nvidia cores</td>
</tr>
<tr>
<td>CINVESTAV</td>
<td>México</td>
<td>SGI ICE-XA (CPU) and SGI ICE-X (GPU) with 8,900 cores and peak performance of 429 Tflops. Storage Type Chandelier Seagate ClusterStor 9000 of 1 Pbytes</td>
</tr>
<tr>
<td>CSC-CONICET</td>
<td>Argentina</td>
<td>AMD Opteron cluster of 4,096 cores and 16,384 Nvidia cores, 8,192 Gbytes of RAM, and storage space of 72 Tbytes</td>
</tr>
<tr>
<td>CUDI</td>
<td>México</td>
<td>CUDI cloud computing service</td>
</tr>
<tr>
<td>UBA</td>
<td>Argentina</td>
<td>One cluster with 30 nodes with two AMD 6320, 64 Gbytes of RAM, 24 Tesla K20c, 2 heavy nodes with extra memory (512 Gbytes of RAM each), and 7 nodes with two Intel E5-2630 v4. Another infrastructure consists of 4 nodes with two AMD Opteron 6320 configured to support cloud computing.</td>
</tr>
<tr>
<td>UCR</td>
<td>Costa Rica</td>
<td>Multiple clusters with capacity of ~80 cores CPU, ~25,000 Nvidia cores, and ~1,450 Xeon Phi cores</td>
</tr>
<tr>
<td>UFRGS</td>
<td>Brazil</td>
<td>256-node cluster with 19,968 CUDA cores</td>
</tr>
<tr>
<td>UIS</td>
<td>Colombia</td>
<td>Cluster of 24 nodes (2.4 GHz and 16 Gbytes RAM) for training activities, and cluster with 128 Nvidia Fermi Tesla (104 Gbytes of RAM and 4 Intel Haswell processors per node)</td>
</tr>
<tr>
<td>Uniandes</td>
<td>Colombia</td>
<td>One cluster with 1,808 cores with HT (8 Tbytes RAM) jointly with 160 Tbytes storage</td>
</tr>
<tr>
<td>National Supercomputing Center</td>
<td>Uruguay</td>
<td>Cluster-UY infrastructure; 29 nodes with 576 cores and 1.28 Tbytes of RAM, and 128 Xeon Phi cores with 16 Gbytes of RAM</td>
</tr>
</tbody>
</table>
This freely accessible infrastructure already in production will be federated thanks to RICAP and will ensure achievement of the network’s objectives. Up until now, access to major supercomputers was limited to only a few countries and groups in the region, but RICAP is expected to change this situation and leverage access to this valuable resource.

It should be borne in mind that RICAP is made up of companies and resource providers (the groups listed above), but also direct suppliers of use cases (BSC, CIEMAT, CINVESTAV, CSC-CONICET and its associated institutions, LAGO and UCR) that will carry out the initial tests of the strategic infrastructure and that will later participate in calls for accessing HPC resources or directly use the network cloud. All resource providers have extensive experience in the tasks related to RICAP, both on the exploitation and federation of computer infrastructures and on R&D work, and together with the other institutions form a balanced consortium between consolidated and emerging groups. Also, they have a wide baggage of participation in FP7 and H22020 projects in the e-Infrastructures sector.

The aforementioned infrastructure is complemented by the availability of a desktop cloud that can be used as training or development platform. This platform allows the creation of virtual clusters that can reproduce any software environment and make it possible to deploy such environments on desktop computers, even while there are end users (students) running their applications. In this way, institutions with no HPC facilities might work with the same software stack used by RICAP providers and be able to teach or test applications and, in some cases, get the results they are looking for.

Work Plan

Below is a brief list of the activities and milestones that have already been or are expected to be achieved during the 2017–2020 period and are of interest to the different user groups in Ibero-American universities and other scientific and technological entities.

2017:

- Federation and production of the strategic cloud infrastructure
- Design of the first call for access to HPC infrastructure and implementation of the web form, associated dissemination and outreach of the call, award of computing resources and use of the infrastructure by the selected groups
- Integration into the infrastructure of the new efficiency solutions provided by RICAP
- General RICAP dissemination and outreach activities

2018:

- Update and operation of the HPC and cloud infrastructures
- Analysis and debugging of possible errors derived from the first HPC call
- Analysis of the results obtained by the new solutions
- Completion of the second HPC call
- Implementation of new solutions combining use of tools in the cloud with accelerators
- General RICAP dissemination and outreach activities

2019:

- Update and operation of the HPC and cloud infrastructures
- Analysis of the results obtained by the new solutions
- Completion of the third and fourth HPC calls
- Implementation of new solutions combining use of tools in the cloud with fault tolerance techniques
- General RICAP dissemination and outreach activities

2020:

- Update and operation of the HPC and cloud infrastructures
- Analysis of the results obtained by the new solutions
• Completion of the fifth and sixth HPC calls
• Implementation of new solutions devoted to computational efficiency with containers
• General RICAP dissemination and outreach activities

Note that the network will be managed through an executive committee formed by a representa-
tive of each RICAP group. The committee will meet remotely once a month as well as face-to-
face once a year. This executive committee will appoint experts to evaluate applications for ac-
cess to HPC resources.

The first RICAP call for requesting computing resources launched in June 2017.

EXPECTED RESULTS

During the initial four years of RICAP, it is expected to achieve multiple milestones and results
that will improve various scientific-technological and social aspects.

Benefits and Expected Impact for Latin America

Strategic infrastructures such as PRACE and EGI (FedCloud) in Europe or the Spanish Super-
computing Network in Spain have had enormous success and a notable impact on the scientific
community in their regions of influence, granting access to large computing facilities to any re-
searcher or group with a need for computational services as long as it presents a project of qual-
ity and interest and is technologically feasible within the capabilities offered.

For this reason, it can be assured that RICAP will have at least as much benefit and impact in
Latin America. And in social terms, its impact will be even greater because it will make availa-
ble to researchers and groups a computing capacity that, in their countries, can be practically im-
possible to materialize. Some of the countries that participate in RICAP have world-class
supercomputing facilities, but some others do not; therefore, RICAP offers these researchers the
opportunity to enjoy this computing capacity for free.

Moreover, RICAP is open to all scientific, technological, and social fields and will be able to
serve—on equal terms—users of any Ibero-American country. Therefore, it offers a clear com-
mitment to social equity. Also, as indicated above, a mechanism will be articulated so that more
Latin American institutions can be integrated into the activities of the thematic network.

Some users have already been preidentified and will be able to use the RICAP capabilities from
the outset. Based on the experience of its founding partners, such as BSC, CIEMAT,
CINVESTAV, CSC-CONICET (and its associated institutions such as CNEA or UBA), and
LAGO, tests will be carried out in areas such as wind energy, medical physics, nuclear and radi-
ological safety, plasmas physics, geophysics, air pollution, radar network design, and wireless
communication.

Also of note is the participation of LAGO,14 which has a working group that specializes in simu-
lation that ensures use of the HTC network for studies of cosmic rays and their effect on the
health of air crews and travelers. LAGO will also apply to access the HPC resources under com-
petitive concurrence.

Thanks to the capacities and solutions provided by RICAP, all these communities will have the
chance to approach the solution of ambitious and complex problems that could not otherwise be
attempted by many Latin American researchers.

Training

Training is a cornerstone of RICAP. The network counts among its members the BSC, one of the
PRACE Tier-0 partners. Within the activities of this great European consortium, a wide variety
of courses is organized by its teams, which can be extended to Latin America with funds from
the PRACE consortium itself. The one- or two-day theoretical-practical seminars that emerge
from this collaboration with PRACE will serve as training for staff developing their work in the HPC/HTC field, a fact that will increase their employability.

In addition to these PRACE courses, there will also be seminars within the academic program directly focused on the use of the strategic network provided by RICAP. These tutorials will be organized in conjunction with events and conferences held in Latin America, such as TICAL, CARLA, and ISUM.

For these conferences and others, a strong collaboration with RedCLARA has been established. Thus, TICAL has effectively integrated community streaming into its Thematic Encounters program, so people not in attendance can still follow the courses locally.

Courses to be taught as part of RICAP include the following:

- access and use of computational resources provided by RICAP,
- understanding high performance computing cluster management,
- hands-on introduction to HPC (PRACE),
- message-passing programming with MPI (PRACE),
- Intel MIC and GPU programming (PRACE),
- methodologies for efficient execution of tasks in HPC and HTC environments,
- performance analysis and tools (PRACE),
- an HPC-CSC intensive school, and
- an SC-CAMP supercomputing and distributed systems camping school (SCCAMP Consortium).

As the list shows, this training plan is designed to encompass and be profitable for different academic levels.

Another important point to note is that the courses and seminars taught within RICAP will be promoted by the academic entities of the network within its degree and master’s courses to encourage attendance by not only computer science students but also students in other departments (science, engineering, statistics, and so on) to whom knowledge of the network is applicable.

LAGO also has its own human resources training program in which the teaching activities of RICAP will be promoted.

To complement training and dissemination activities, several events are regularly organized in Argentina, Uruguay, Brazil, Costa Rica, Mexico, Colombia, and other Latin American countries. The High Performance Computing School (ECAR) and the International SuperComputing Camp are two examples. With respect to networking activities highlighting HPC in Latin America, WHPCEuroLatam is periodically allocated as part of ISC-HPC, and an Americas HPC Collaboration BoF was recently held as part of Supercomputing 2017.

All didactic materials generated (presentations, exercises, videos) will be posted on the network webpage and made permanently available for free on the RICAP website (http://www.red-ricap.org).

CONCLUSIONS

By making a huge amount of computational resources freely available, RICAP will generate a multitude of new activities in different scientific and social areas of Latin American society. This is particularly significant today, with computing so hugely integrated into the generation of scientific, social, and engineering knowledge in both the public and private sectors. It will also contribute toward improved social equality because access to the infrastructure will be direct (cloud) or competitive concurrency (HPC) based, meaning that scientific interest will prevail and end users without local access to HPC and HTC environments will be able to carry out their work.

The originality of the network lies in the fact that regional access is not a reality in Latin America as a whole, but only at a national level in some countries. Therefore, RICAP represents a tremendous advance for scientific communities across all areas in the region.
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