High-Performance Computing in Materials Science

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Abstract

Computational modeling in materials science involves the employment of fundamental physical and life sciences as well as computer science to study the properties of matter at the microscopic level. Such studies can be carried out by electronic or atomistic approaches and the outcomes used to complement the applied sciences as well as to guide experimental research work. Over the last decade, affordable computing resources coupled with community developed state-of-the-art codes are available for graduate students and research staff even in the developing world, where there is limited funding. This has been made possible through collaborative research or via initiatives from friendly partners in Europe and America. It is, therefore, possible to engage in quality research for capacity building or the development of products and services. Computational modeling can now predict, independently, outcomes of some materials properties to within accuracies of less than 5% compared with independent experimental techniques. This implies that computational modeling can be used as a decision support tool, enabling tests before production, hence cutting down costs from the previous trial and error approaches. Current problems in science and technology require a multidisciplinary approach such as that being employed in computational modeling and hence its applications in both fundamental and applied sciences. Due to the accessibility of resources to perform research using computational modeling in materials and other applied sciences, additional effort needs to be made to involve more graduate students and faculty in these areas for capacity building. In due course, it is expected that the research capacity realized will be focused to solve current and emerging problems in this country.

1.0 Introduction

Computational modeling in materials science is the use of computer science, fundamental biology, chemistry, mathematics, and physics to study the properties matter. Research studies in materials science that can benefit from computational modeling include both fundamental and the applied sciences. High-Performance Computing (HPC) is the application of dedicated and coordinated computer resources over a period of time to solve research problems that require massive computer speeds and memory. Computational modeling has evolved from traditional and basic problems to a state-of-the-art technique used as a decision support tool in materials science research. The results of carefully thought out and executed research problems are informative as well as accepted by the scientific community through dissemination in presentations and peer-reviewed journal publications.

Graduate students and academic staff in countries where there is limited or no funding for experimental approaches to carry out research as well as research groups that have standard and well maintained experimental infrastructure who need results of simulations of their systems to seek insights into their work are likely to greatly benefit from this approach. A beginner requires a standard desktop computer with 2 – 8 Mb Ram, at least 500 Gb of hard disk space or a laptop of similar specifications with basic computer knowledge. Having a laptop has the advantage of easy movement to interact with others. While having a windows operating system to take advantage of free software is sufficient, graduate students and younger faculty are strongly encouraged to have open-source operating software installed in the desktop or laptop. It should be noted that most software running on the open-source system are free and do not require a license. A learner should be prepared to invest at least three months to be comfortable with navigation on the open-source system and to learn to use basic system commands in order to run beginner calculations on properties of well-known materials. Competence beyond that, even at the first-degree level, requires more investment in time but leads to comfort in the understanding of scientific concepts and interpretation of results.

2.0 Resources needed for research engagement in computational modeling in materials science

To undertake research on larger problems that require additional computational resources above a desktop/laptop one has to look to other providers. At the national level, The Kenya Education Network (KENET) provides graduate students and faculty-specific cloud services and training with arrangement for calculations [1]. The African School on Electronic Structure Methods and Applications (ASESMA) series is a biannual event held on the African continent supported by the host African government as well as several international partners [2, 3]. This 2 weeks School provides intensive free training in the theory and hands-on experience and is highly recommended for graduate students and young faculty.

The largest provider of dedicated remote computational resources in science, technology and innovation is the Department of Science and Technology of the Republic of South Africa, through the Centre for High-Performance Computing in Cape Town. Depending on personal interest it is possible to join an existing research group. Kenya, being part of the global Square Kilometre Array (SKA) consisting of 9 African countries, has access to the computational resources at the CHPC [4]. The CHPC has research groups working on both fundamental and applied sciences. There are less than 10 Kenyan researchers who are registered as principal investigators at the CHPC but who can grant access to the resources provided one has a well defined research problem to investigate. There are global enterprises such Amazon and Microsoft Azure that are ready to get researchers and graduate students to test their computing resources in science, technology and innovation as well as other fields but have charges after a trial period.

It is possible that before 2008, there were graduate students and faculty engaged in computational modeling in fundamental and applied sciences in Kenya but the efforts were scattered. Beyond this period the initial institutional support from Moi University, the National Council for Science Technology and Innovation (NACOSTI, then National Council for Science and Technology), the International Centre for Theoretical Physics (ICTP, Trieste, Italy) enabled the first visibly coordinated research work in materials science research work through computational modeling. Later, support from University of Eldoret, ASESMA, the Emerging Nations Science Foundation (ENSF), the German Academic Exchange Service (DAAD), The Academy of Science of Developing Nations (TWAS), among other well wishers, enabled the growth of training and mentorship of graduate students as well as faculty. In May/June, the second ASESMA event in Africa was held in Kenya, in then Chepkoilel University College (now University of Eldoret) (See Figure 1 showing participants). Since then, materials science modeling in Kenya has been rated as only second to South Africa in African in terms of productivity in graduate student training and international peer reviewed publications [5].

Figure 1: Participants of 2nd ASESMA event in May/June 2012.

The initiatives in University of Eldoret received a direct support from the ENSF that was channeled to support meritorious undergraduate students in their final year between 2013 and 2017, graduate and postdoctoral students in a mentorship program aimed at preparation for graduate school and research. It is worth noting that just based on merit, the students who went through the program came all over the country (See table 1).

Table 1: Details of the mentees of the program and progression.

	Name (gender)	Entry level/ discipline	Area	Current status
1	Moro, Cecil	Undergrad /Physics	Comp. Mat. Sci	Phd/Physics – University of Pretoria Research Associate (CSIR, South Africa; HySA NWU, South Africa)
2	Mwonga, Patrick	Graduate	Comp. Mat. Sci	PhD/School of Physics Wits (Gauteng, South

		Msc/Physics		Africa)
3	Mutisya, Sylvia (F)	Undergrad /Physics	Comp. Mat. Sci	Phd/Physics - Brazil Postdoc/Physics Saclay, France
4.	Muchiri, Perpetua (F)	Undergrad /Physics	Comp. Mat. Sci	Msc/TU-K Graduate Assistant (TU-K)
5	Ochieng, Edmund	Undergrad /Computer Science	Cluster and Software support	System Admin at Rackspace Hosting (Texas, USA)
6	Mwalukuku, Valid	Undergrad /Chemistry	Comp. Mat. Sci	Msc/Chemistry Grenoble, France
7	Aradi, Emily (F)	Undergrad /Physics	Comp. Mat. Sci	Postdoc/Physics (UK)
8	Atambo Michael	Undergrad /Physics	Comp. Mat. Sci Cluster and Software support	PhD/Physics (Modena University, Italy) Lecturer, TU-K
9	Buko, Eric	Undergrad /Physics	Comp. Mat. Sci	PhD/Medical Physics (Texas, USA)
10	Ruggut, Elkana	Undergrad /Physics	Comp. Mat. Sci	PhD/School of Physics Wits (Gauteng, South Africa)
11	Korir, Kiptiemoi	Graduate PhD/Physics	Comp. Mat. Sci	Phd/Physics – Torino, Italy Lecturer, Moi University College, Busia
12	Meng'wa Victor	Graduate MSc/Physics	Comp. Mat. Sci	PhD/Physics UoE/OFID_ICTP/TU-K Lecturer, Alupe University

				College

Research activities in materials science at the national level are now supported by the Kenya Education Network (KENET) under the Computational Modeling and Materials Science (CMMS) special interest group. CMMS has over 70 research active Kenyan graduate students and faculty representing fundamental and applied sciences. KENET recently competitively awarded five mini grants to 5 Kenyans from public and private universities to carry out research on the areas of materials for green energy conversion and environmental safety.

3.0: Achievements and the need to focus on local problems

Following the growth of the group on Chepkoilel University College and later University of Eldoret, new groups have emerged in Masinde Muliro University of Science and Technology as well as Egerton University led by newly acquired PhDs who were part of the original vision. Through active collaborations, a group in Kabarak University is also now in its formative stages. It is estimated that through efforts to introduce high performance computing in materials science about 6 Phds and 15 Msc students have been trained since 2010 from University of Eldoret alone and much more at the national level.

For such knowledge and output to have an impact to the common citizens, a paradigm shift from publishing for its own sake or for promotions is needed. Graduate students and younger faculty should now go out to industry to seek current and emerging problems that have value to the country.

4.0: Conclusion and recommendations

Computational modeling in materials science is a research direction that can be used to investigate problems in fundamental and applied sciences giving high quality results. The largest informational impact on the use of the approach is realized when the approach is employed as a complementary check on experimental research work and also to provide predictive insights.

Institutions in Kenya, especially those previously shying away from fundamental and applied sciences, are encouraged to invest resources in this area in order to effectively use this approach for student and faculty training. There is an over reliance on the support from the Republic of South Africa for computational resources but it is my hope that the Government of Kenya will make an investment in local infrastructure for Kenyans undertaking research that will target projects of national strategic value using this approach.

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