Contribution ID: **24** Type: **Abstract for Research Paper**

High Performance Computing in Materials Science

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.

Keywords

High Performance Computing, Materials Science

Primary author: AMOLO, George (The Technical University of Kenya)

Track Classification: Computational Modelling of Materials