Call for Proposals
Computational Modelling and Materials Science Grants - 2022/2023

KENET Research and Innovation Grants Overview

KENET has as one of its mandates, the role of catalyzing collaboration in research and education among member universities and research institutions. KENET promotes collaboration through facilitation of Special Interest Groups (SIGs) in priority academic areas, discovery of active researchers/faculty, provision of research and education grants to researchers and member institutions, as well as travel grants for faculty and/or graduate students in the SIG areas.

KENET operates a research cloud (https://vlab.ac.ke) that provides free research computing and storage services to doctoral students, faculty, and researchers. KENET also facilitates access to HPC facilities by researchers and grantees when required.

The Computational Modelling and Materials Science (CMMS) is one of the Special Interest Group supported by KENET to enhance research capacity development in the use of computational modeling in science and technology. Research grants support the research projects of early career PhD faculty and researchers in computational biology, chemistry, mathematics, physics, environmental and engineering sciences. In order to increase the research output from research groups with standard experimental infrastructure, CMMS has embraced computational modeling which is now considered an important decision support tool. In this regard, CMMS research team must include graduate students, preferably PhD students. Teams can also include industry researchers working in innovation hubs or startups.

In the past two years, KENET has supported five university-based SIG in CMMS research teams from six different universities with a grant of KES 1.5 million. In addition, KENET has awarded to grantees in engineering and computer science and information systems SIGs. (see https://www.kenet.or.ke/content/call-proposals-computer-science-information-systems-and-engineering-multi-disciplinary-0)

KENET invites proposals from the SIG CMMS in the following focus areas:

1. Modelling in Bioinformatics, Computational Biology and related fields.
2. Materials modelling for energy conversion and related areas.

KENET plans to award three catalytic research grants of KES 1.5 million to successful SIG CMMS grantees.

CMMS Grants: Structure, Technical Brief and Schedule

Grants Structure

1. Three (3) grants will be awarded for the 2022/2023 round of funding.
2. Each research grant will be for a maximum of Ksh1.5M.
3. The team leader must be a faculty member who obtained the PhD degree less than six years from the date of this Call for Proposals.
4. Research teams are encouraged to include doctoral students in their second or third year of PhD research.

Areas of Focus: Technical Brief

1. Modelling in Bioinformatics, Computational Biology and related fields

Computational Biology and Bioinformatics are fields that develop and apply computing techniques to investigate biological systems such as genetic sequences, cell populations or protein samples as well as drug design and the exploration of other novel biological phenomena. These are important in understanding genetic information that define human diseases as well as drug design, among others. The recent advent and social economic disruption caused by the Covid19 pandemic has exposed the need to have more local technical know-how in these areas and thus minimize reliance and direction from the developed world. The computational techniques used include mathematical modeling and simulation, analytical methods, all of which enable the qualitative and quantitative analysis of the biological systems, thus allowing interpretation and exploitation. These thematic areas will advance the country's goals towards provision of healthcare through local and affordable drug development as well as a safer environment which should resonate well with Kenya's big 4 agenda.

2. Materials modelling for energy conversion and related areas.

This theme involves the application of computer clusters and codes to simulate the structural (geometry, hardness/strength), electronic (band gaps, transport, magnetic) as well as the optical properties of bulk materials, 2D and nano-materials, be they organic or inorganic, using *ab initio* or suitable empirical approaches.

Employing these codes to investigate materials of interest provides information in fundamental (Chemistry, and Physics) and applied (chemical, electrical and mechanical engineering, among others) sciences that enables users to undertake research in current as well as emerging areas in their field of interest. Decreasing costs and increased computing power has now enabled simulations of systems of a few hundred atoms edging closer to the physical reality. New codes currently enable simulations to take a predictive rather than complementary role, which is important in guiding experimental work and indeed production of new materials, minimizing trial and error that have characterized past research. This theme targets the development of knowledge and skills in the areas of materials for energy conversion and related areas.
Those intending to employ both experimental as well as computational modeling approaches by seeking appropriate collaborations should provide the necessary detail and may have an added advantage.

SIG in CMMS research grant call timeline:

Activity	Dates
Call for proposals open for submissions	4th February 2022 to 4th March 2022
Review and evaluation of received proposals	7th – 25th March 2022
Face-to-face presentations of shortlisted applicants	30th March 2022
Finalists announced and grants awarded	4th April 2022
Grantees on-boarding	11- 14th April 2022
Implementation period	14th April 2022 - 14th April 2023
Evaluation, monitoring, reporting and close-out	E & M – quarterly per group

CMMS Grants: Eligibility, Terms and Conditions

Eligibility

This call is open to computational modeling and materials science faculty (who are full-time) at any of the KENET member institutions. The lead applicant must be a PhD holder, attained within the last 6

years, and must demonstrate active research interest.

Recent KENET grantees of Computational Modeling and Materials Science (CMMS), Computer Science and Information Systems (CSIS) and Education Technologies and Engineering (ETD) are not eligible to apply.

Team Composition

The lead researcher(s) must be a PhD holder meeting the eligibility criteria above. The lead researcher is strongly encouraged to incorporate other researchers, including senior colleagues, into their team, especially dedicated research staff or full time MSc/PhD students. If other members are incorporated into the team, then the roles and extent of involvement of these team members must be clearly spelt out. A letter of Commitment from each Team Member with support from respective Heads of Department or Deans, must be included as part of the team's submission documents. In this letter, each organization or individual must submit in writing their commitment to participate in project activities, specifying their exact role in the project. Teams with multidisciplinary backgrounds are encouraged. The lead researcher will serve as the team leader and the primary point of contact for the team on all matters related to implementation of the grant.

Student Involvement

One of the main objectives of this grant is to develop expertise and build capacity in the areas of focus, and to grow a community of practitioners. To this end, it is important for faculty to work closely with students with a view to furthering their knowledge and capacities in the various technologies and issues of interest, in the areas of focus. Incorporating students as team members as well as designing student-level projects from the research activities to be undertaken is encouraged.

Collaboration and partnerships

To enhance research uptake and utilization, it is important for researchers to identify and seek out collaborations and partnerships with strategic persons and institutions. This not only opens up pathways for moving research from the lab to the society, but also enhances visibility of researchers and their institutions, attracting even more funding and opportunities to further their research agenda. Given the identified areas of focus, it will be imperative for teams to identify strategic partnerships and collaborations with a view to modeling and planning for prototyping, testing and scaling at later stages in the research cycle.

Intellectual Property

Intellectual property derived from the funded R&D activities will be appropriated and protected based on the lead researcher's institution's IP policy and procedures.

Post-Award Requirements

The successful grantees will be expected to:

1. Provide quarterly progress reports to the CMMS Research Associate at KENET.
2. Participate and present project work at selected meet-ups organized by KENET.
3. Grow a community of researchers in the area, by reaching out to other local researchers working in the area and other related multidisciplinary domains
4. Actively seek post grant funding to further their research work by writing (joint) funding proposals
5. Prepare a final project report at the end of the grant period and submit to KENET. Prepare an abridged version of the project report for profiling on KENET's and institutional websites.
6. Publish paper(s) on their work in reputable journals.

CMMS Grants: Proposal Submission

Concept Note Format

1. The concept note should not exceed 6 pages (12pt, single spacing, excluding appendices).
2. The concept note should be submitted in PDF format.
3. The research area should be clearly indicated in the title page.
4. No personal identification (names) or institutional affiliation should be included in the concept note.

Concept Note structure

The concept note should have the following structure:

1. Title
2. Problem definition and justification
3. Proposed solution and justification
4. Methodology
5. Resources (human, hardware, software etc.)
6. Work plan (not exceeding 12 months in duration)
7. Detailed Budget (not exceeding Ksh1.5M)
8. Appendices

Supporting Documents

The following documents should be included as part of the concept note submission:

1. Team profile document, indicating the names, institutional affiliation and brief biographies of the lead researcher(s). Details of other team members and any collaborating institutions should also be included in the team profile.

2. CVs of the lead researcher(s), clearly profiling research activities undertaken to date as well as relevant publications.
3. Letters of Commitment from team members and any collaborating institutions.

Concept Note submission

Concept notes with all supporting documentation should be sent via email to cmmsgrants@kenet.or.ke by March 4, 2022.

Enquiries and applicant support

All enquiries and requests for further information related to this call should be addressed to grantsadmin@kenet.or.ke.

CMMS Grants: Proposal Evaluation

1. KENET will constitute a review panel of leading CMMS experts. Members of the review panel will sign Non-Disclosure Agreements, as well as statements acknowledging that they will make no claim to the intellectual property developed by the grantees.

2. The reviewers will review all received applications as per the evaluation criteria provided in the table below, and select the top 3 proposals for each area of focus.
3. The top three (3) finalists in each area will be invited for a final face-to-face presentation. During the oral presentations, the applicants will respond to and clarify any questions from the panel that will have arisen out of their written submissions. They will also be required to respond to any ad-hoc questions arising from the oral presentation.
4. After the oral presentations, the reviewers will make their final decisions on which one

proposal will receive the grant, per area of focus. Three (3) teams will be selected.

5. Selected grantees will be notified formally and profiled on KENET's website.

Evaluation criteria:

Evaluation Criteria	Evaluation Aspects	Weighted Score
Relevance and justification of proposed research topic	Is the proposed topic and preferred solution aligned with Kenya's Big 4 agenda, Vision 2030 or SDGs? Is it an important problem to solve in a developing world context? Is there sufficient research uptake and utilization potential for the proposed research outputs?	15%
Technical Approach and Methodology	Is the research concept innovative and effective compared to existing alternatives? Does the proposed approach have a potential experimental component partner to test the computational findings proposed? Is there a potential HPC development component? Is the proposed work doable given the time and budgetary constraints of the grant, considering the team's composition?	35%
Budget justification	Are the items to be procured related to the project objectives and activities? Can these items be obtained within the project timelines?	10%
Viability assessment and scaling potential	Is scale built into the solution? Can it be replicated in similar contexts? Is there scope for furthering the research idea/prototype? Is there scope for future external research funding in order to scale-up the research?	10%
Human capacity	Does the team have the required expertise, experience and necessary contacts to deliver? Do they have a local footprint?	10%
Student engagement	Are there concrete roles and responsibilities for student team members? Are there clearly defined student-level project ideas?	10%
Inter-university/industry involvement	Have critical partnerships in the main domain of application been identified? Is there likelihood for collaboration during and after the grant period? Does lack of partnerships severely impede the research work during the grant period?	5%
Potential for publication in refereed journals and/or conferences	Are the results likely to be published in international peer reviewed journals / conferences that are indexed in Elsevier Scopus database?	5%