

Call for Proposals

Research and Innovation Grants in Computational Modelling and Materials Science Grants - 2023/2024

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 SIG areas.

The Computational Modeling and Materials Science (CMMS) is a special interest group supported by KENET to enhance research capacity development in the use of computational modeling in science and technology. Research work is expected to involve university faculty and graduate students in Biology, Chemistry, Physics and the Environmental sciences but strongly welcomes those from other basic and applied sciences. To increase research output directly or by complementing the existing limited work from groups with standard experimental infrastructure, CMMS has embraced computational modeling which is now considered as an important decision support tool in science and technology as well as product development. In this regard, CMMS targets training of graduate students as well as young and upcoming faculty in universities, research institutions and industry.

KENET has provided CMMS with Four (4) grants of Ksh 1.5 Million each, to be awarded competitively in the following computational modeling themes:

1. Bioinformatics and Biochemistry applications.
2. Earth observation science and technology.
3. Materials for energy conversion using basic and applied sciences

Innovation Grants: Structure, Technical Brief and Schedule

Grants Structure

1. Four (4) Research and Innovation grants will be awarded for the 2023/2024 round of funding.
2. Each grant will be for a maximum of Ksh1.5 Million
3. The grants period is 12 months.

Areas of Focus: Technical Brief

1. Bioinformatics and Biochemistry Applications

Computational Biology and Bioinformatics is a relatively new scientific field that develops and applies computational techniques to study biological systems such as genetic sequences, cell populations or protein samples as well as drug design and the exploration of other novel biological phenomena. This field is important in understanding genetic information that defines human diseases as well as drug design, among others. 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. This thematic area will advance the country's goals towards local and affordable vaccine/drug development as well as a safer environment which should resonate well with Kenya's big 4 agenda. Applications will be considered for, but not limited to:

- a) Vaccine development in the country,
- b) Genetically modified plants that resist chemicals added to the soil.

2. Earth Observation Science and Technology

Human development and sustainable utilization of natural resources requires a balance in order to ensure that the next generation inherits a habitable world. In recent years, Earth Observation Science and Technology has taken a firm root in providing information on the state of planet earth thereby generating large volumes of data that require careful collection and storage. Information accessible is provided by satellite, lately also involving drones, with image capturing devices and includes the physical, chemical and biological state of the earth. Such data provides a space map on activity on the ground from agriculture, mining, water management, forestry, as well as rural and urban growth, among others. Earth Observation Science and Technology can be used to support policy development by national and local authorities, sustainable commercial exploitation and innovation by industry as well as ecological and biodiversity protection for posterity. Applications will be considered for, but not limited to:

- a) Applications in agriculture and climate change,
- b) Use of Unmanned Aerial Systems(UAS) for data collection.

3. Materials modeling for energy conversion using basic and applied sciences

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 as well as nano-materials, be they organic or inorganic, using *ab initio* or empirical approaches. Employing these codes to investigate materials of interest provides information in basic (Biology, Chemistry, Mathematics and Physics) and applied (chemical, electrical and mechanical engineering) sciences 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. Applications will be considered for, but not limited to:

- a) New materials for battery and supercapacitor applications,
- b) Phase change materials for thermal storage.

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.

Using High Performance Computing (HPC) cluster for computational modeling to solve problems in science and technology.

Simulations to study real systems for possible applications require computing resources beyond laptops and desktop computers. This calls for computing capacity that is dedicated to perform tasks that require large resources with calculations which run continuously with minimal interruption. Kenya does not have a national HPC facility for basic and applied sciences to support research that could benefit from computational modeling. In many cases, researchers undertaking

work that requires intense calculations for a long period of time rely on supercomputers provided by collaborating institutions in other parts of the world.

KENET provides a select set of computing services to the grantee's that includes access to computing facilities at partner institutions, such as the CHPC, as well as 24 hours local cloud services, that may be used as a platform to power computational needs of the research problems. All these are tailored towards development of HPC capacity, and efficient utilization of the same in the local research fraternity. These computing skills should enable the application of novel computational methods such as machine learning, both CPU and GPU based, to aid in innovation and design.

Applicants in these areas should consider the calls by KENET for support as preparation for funding to other organizations, at the national and international levels, providing much larger support.

Eligibility, Terms and Conditions

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 5 years, and must demonstrate active research interest. Those recently awarded grants from the Computer Science and Information Systems (CSIS), CMMS and Engineering are not eligible to apply. Candidates who have received their PhD from Kenyan institutions may have an added advantage where applicable.

Team Composition and 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. The lead researcher(s) must be a PhD holder meeting the eligibility criteria above. The lead researcher is strongly encouraged to incorporate other researchers 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. Teams with multidisciplinary backgrounds are encouraged. The lead researcher will serve as the team leader and the primary point of contact on all matters related to implementation of the grant.

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 it 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.

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 i.e.
4. To enable a blind review process, 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 (Ksh1.5 Million). Only up to 40% of the total budget should be set aside for purchase of PCs, laptops. The use of the KENET cloud services is strongly encouraged.
8. Relevant 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 **14th July 2023, 5.00PM EAT**.

Enquiries and applicant support

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

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 Table 2 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 the proposals that 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.

Table 2: 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 with 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 the Elsevier Scopus database?	5%