



Call for Proposals

Computational Modeling and Materials Science Mini-Grants 2018/2019

KENET's Mini-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, and provision of research and education mini-grants to researchers and member institutions, as well as travel grants for faculty and/or graduate students in SIG areas.

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 within this group is expected to involve university faculty and graduate students in 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 research infrastructure, CMMS has embraced computational modeling which is now considered as an important decision support tool. In this regard, CMMS targets training of graduate students as well as young and upcoming faculty in universities, research institutions and industry.

CMMS has been provided with 3 mini grants of USD15000 each, to be awarded competitively in the following themes

1. Materials modeling and development for energy conversion using basic and applied sciences
2. Materials science and technology for environmental safety and health applications

CMMS Mini-Grants: Structure, Technical Brief and Schedule

Mini-Grants Structure

1. Theme 1 will be awarded two (2) mini-grants with theme 2 having one (1). A total of three (3) mini-grants will be awarded for the 2018/2019 round of funding.
2. Each mini-grant will be for a maximum of 15,000 USD.
3. The grant period is 12 months.

These grants should provide a platform for preparation to seek larger funding from other organizations as well as attract collaboration from both local and international partners.

Areas of Focus: Technical Brief

1. Materials modeling and development for energy conversion using basic and applied sciences

This theme involves the application of fundamental science and computer clusters as well as 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) 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, minimizing the trial and error that have characterized past research as well as the cost of production of new materials. The focus here is the development of knowledge and skills in the area of materials research for energy conversion and related aspects.

Those intending to employ both computational modeling as well as experimental approaches by seeking appropriate collaborations should provide the necessary detail and may have an added advantage.

2. Materials science and technology for environmental safety and health applications

Computational modeling to investigate and complement research on environmental factors that impact our wellbeing is vital in this age of industrial and fuel pollution that has affected the air as well as the quality of water resources for domestic use, aquaculture and agriculture. The flow of water below the surface of the earth can also be usefully studied through simulations thus empowering hydrological related research.

Involving scientific computing is essential to study the solid earth since large depths regions close to the centre of the earth are not easily accessible to experimental investigations but the high pressure and temperature conditions can be simulated. Information from such studies is fundamental to the practical areas of seismology and mineral formation research for correlation to independent data obtained from the earth, hence informing investment opportunities and other social economic activities.

This theme is open to interests in environmental safety, wellness and mineral formation in solid earth, hence targeting applications in water purification, drug design chemistry, mineralogy and related application aspects. Collaboration with other institutions or industry is strongly encouraged.

CMMS mini-grant Call timeline:

Activity	Dates
Call for proposals open for submissions	18 th December 2018 to 15 th February 2019
Review and evaluation of received proposals	22 nd February - 8 th March 2019
Face-to-face presentations of shortlisted applicants	11 th March 2019
Finalists announced and mini-grants awarded	12 th March 2019
Grantees on-boarding	13 - 15 th March 2019
Implementation period	1 st April 2019 - 31 st March 2020
Evaluation, monitoring, reporting and close-out	E & M – quarterly per group

CMMS Mini-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 5 years, and must demonstrate active research interest. Those recently awarded mini-grants from the Computer Science and Information Systems (CSIS) 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 at liberty to incorporate other researchers into the team as needed. If other members are incorporated into the team, then the roles and extent of involvement of these team members must be clearly indicated. 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 mini-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 mini-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 Mini-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 i.e.
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 15,000 USD)
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 submitted online by 15th February 2019, 5.00PM EAT. The URL for submission is <https://www.kenet.or.ke/call-for-mini-grants-proposals-2018-2019>

Enquiries and applicant support

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

CMMS Mini-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 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 which proposals will receive the mini-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:

<u>Evaluation Criteria</u>	<u>Evaluation Aspects</u>	<u>Weighted Score</u>
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 mini-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? Has the team been involved in similar work?	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%