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EUE Proposal

Project ID#

2020-01

Project Title

Scaffolded Projects for Applied Numerical Science, Part of a new course in computational science for STEM students

Project Director	ID Number	Telephone	Email
Edward Ackad	800475119	6186502390	eackad@siue.edu

Department	Campus Box	School College
Physics	1654	CAS

Course or Program

Physics 219: Applied Numerical Science

Project Co-Director	ID	Department	Email

Student Impact:	Est. 40/year

Priority Rating (If Submitting Multiple Proposals):	

Project Budget

Salary	Wages	Travel	Equip.	Comm	CServ	Auto	Tele	Awards	Total
7116	1637								8753

Cost-Sharing

Salary	Wages	Travel	Equip.	Comm	CServ	Auto	Tele	Awards	Total

Prior EUE Support

Project Director	Project Number	Award Amount	Project Dates

Project Summary
I am excited about my newly designed class for the physics department on Computational Science that will teach STEM students how to solve problems from many areas of science algorithmically, model systems, program, plot, and visualize data in Python. This award will be used to create and refine six scaffolded computational science projects for the upcoming Physics 219 "Applied Numerical Science" course as well as prepare, submit, and setup the computational infrastructure needed for students in the course. This award will deliver: (i) an educational allocation on the JetStream Cluster (part of XSEDE), (ii) a template for future educational allocations on JetStream, (iii) a simple environment with all the needed software for students to use in the class accessible from anywhere using a web browser, and (iv) four tested and refined scaffolded projects that students will work to complete. The projects will allow students to gain hands-on learning in small steps and focus on the relevant topics since other topics will be already in the scaffolded code. Additionally, these projects will include a full write up explaining the modeling used, mathematics needed, science background, and programming concepts used. Using the jupyter system, teams of students working together will plot and visualize their results in different ways to gain an understanding for all aspects of the problem (theoretical modeling, mathematical modeling, computational implementation, and the meaning and limitations of their results).

Biographical Sketch for Edward Ackad

A. Professional Preparation

Undergraduate Concordia University	Physics	BSc 1998-2002
York University	Physics	Ph.D 2002-2008
University of Ottawa	Laser-Cluster interactions	2008-2011

B. Appointments

Associate Professor (SIUE)	2017-
Assistant Professor (SIUE)	2011-2017

C. Funding (successfully obtained funding for research and teaching)

Behavior of atoms in strong laser fields, Ministry of Research and Innovation (Ontario)	$100,000 2007-2009
Nanolithography Using X-ray Seeded Plasmas STEP, SIUE	$15,061 2012-2013
Understanding Laser Cluster interactions in the X-ray Regime Air Force Office of Scientific Research	$560,000 2014- 2018
CC*DNI Networking Infrastructure: Dedicated High-Speed Research and Education Network Connection National Science Foundation	$374,093 2016-2018

D. Products (undergraduate co-authors are highlighted)

Soft-Matter

1. The NS4A Cofactor Dependent Enhancement of HCV NS3 Protease Activity Correlates with a 4D Geometrical Measure of the Catalytic Triad Region, Hamzah A. Hamad, Jeremy Thurston, Thomas Teague, Edward Ackad and Mohammad S. Yousef (PLOS ONE under minor revision, expected publication Dec 2016)

2. Comparative Molecular Dynamics Simulation of Hepatitis C Virus NS3/4A Protease (genotypes 1b, 3a and 4a) Predicts Conformational Instability of the Catalytic Triad in Drug Resistant Strains
Mitchell Kramer, Daniel Halleran, Moazur Rahman, Mazhar Iqbal, Muhmad Ikram Anwar, Salwa Sabet, Edward Ackad and Mohammad Yousef. PLOS ONE 9 e104425

3. A 3D structural model and dynamics of hepatitis C virus ns3/4a protease (genotype 4a, strain ed43) suggest conformational instability of the catalytic triad: implications in catalysis and drug resistivity
Bradley Rimmert, Salwa Sabet, Edward Ackad and Mohammad S. Yousef, J Biomol Struct Dyn. 2014 Jun; 32(6): 950–958

Nanophotonics

4. Ultraintense Laser-Cluster Interactions: Effects of the Cluster Shape
Kasey Barrington, Zachary Hartwick, Joseph Trost, Rishi Pandit, Nicolas Bigaouette, Lora Ramunno

and Edward Ackad, Physical Review A 93, (2016) 013417

5. A validation of a simple model for the calculation of the ionization energies in X-ray laser-cluster interactions
Jeff White and Edward Ackad, Phys. Plasmas 22, 022123 (2015)

(ii) Other Significant products

1. Nonlinear grid mapping applied to an FDTD-based, multi-center 3D Schrödinger equation solver
Bigaouette, Nicolas; Ackad, Edward; Ramunno, Lora; Comp. Phys. Comm. **183** (2012) 38

2. Clusters in Intense XUV pulses: effects of cluster size on expansion dynamics and ionization
Edward Ackad, Nicolas Bigaouette, Kyle Briggs and Lora Ramunno 2010 Phys. Rev. A 83 (2011) 063201

3. Augmented collisional ionization via excited states in XUV cluster interactions
Edward Ackad, Nicolas Bigaouette and Lora Ramunno 2011 J. Phys. B 44 (2011) 165102
4. *Calculation of electron-positron production in supercritical uranium-uranium collisions near the Coulomb barrier*
Edward Ackad and Marko Horbatsch 2008 Phys. Rev. A 78 062711

Synergistic Activities

My experience in both computational and theoretical physics research and my experience of *teaching and mentoring* undergraduate students in my research area will make Physics 219 an ideal place for STEM students to learn the basics of how to do science computationally. My publication record with undergraduate students demonstrates I train them to be active research participants using computational tools. Formalizing this into a course will reach many more students and this award will help make the course a true success, not just for when I teach it, but for any instructor.

Additionally, the JetStream virtual machine setup will allow my research students to work outside my lab, if they chose, on JetStream, with the needed software installed. This will forgo the two-three week setup period students tend to go through on their private computers.

a. **Current Situation**

Many years ago, physicists coined the term "the third way" to describe doing science using computation instead of using only theory or experiment. Today computation is found is almost any disciple. Today's STEM students must be able to harness and understand computational modeling in order to work effectively in science. However, current curriculums (SIUE and others) teach some computer programming often does include problem solving using numerical techniques leaving a skills gap

Impact on undergraduate education: Physics 219, *Applied Numerical Science* has been developed by the physics department to fill this knowledge gap. Unlike the introductory courses in computer science which teach the fundamentals of programming and programming paradigms, this course focuses on teaching students programming and algorithmic modeling to solve problems in a wide range of science (e.g. biology: predator prey model, economics: black-scholes pricing, environmental science: wild fire spreading, physics: galaxy formation, etc.). Students from all STEM fields will be qualified to join the course as either a substitute for the computer science introductory programming course or as an elective (note: it cannot be counted as equivalent for students in programs that require a follow-up introductory programming course as the course will not cover the breadth needed, instead focusing on depth and computational problem solving). The course is scheduled to be offered by the PI, Dr. Ackad, in spring 2020 and it is expected to have around 25 students (10 physics majors, a few math and chemistry students, and some engineering students). We expect the population to grow substantially as the engineers find the course more hands-on and directly applicable to their studies.

This award will create the digital "infrastructure" and will thus live on in perpetuity for future offering of the course and include a template application for JetStream (supercomputing time for the students) for future offerings. In short, this award will allow the PI to create the infrastructure that will allow the course to be offered in the future by anyone with well-prepared projects and user shells.

b. **Proposed Project**

This award is designed to allow the PI to create needed material for the Applied Numerical Science in such a way that students without prior programming experience can solve hard science problems starting in their first week of class. This requires (1) well tested and carefully scaffolded starting templates, (2) as well as an easy to access and use "setup" (by which I mean virtual machine, described below).

Students learning to program and then solving problems with programming is a relatively new approach in the undergraduate curriculum. While professional associations such as the American Association of Physics teachers have stated clearly that undergraduate curricula needs more computational science [1-2], the clearest, demonstration for the need of this material is from the National Science Foundation's re-designation of STEM to STEM+C (STEM + Computing Partnerships) which is trying to address the need of educating students in computational (or algorithmic) thinking (on and off computers). Computational (or algorithmic which I find more descriptive) thinking seeks to get students to think about how to solve problems systematically, such as giving the rules on how to play *and win* at Tic-Tac-Toe instead of guessing what to do next for each move. In order to accomplish this effectively with students who have not had any programming experience will require carefully constructed and scaffolded projects that lead the students through the exercise with maximum time spent on the focus of the project and (mostly) ignoring the code segments still beyond them but needed to make the project work and be well visualized.

Detailed Description of the Projects: This award will fund the creation of four scaffolded python-based jupyter-lab. The four projects are expected to be: (1) bungee jumping, (2) Enzyme Kinetics, (3) Global Warming, (4) Markov Chains in genetics. These projects will create first as full solutions with large and detailed comments for all the code and introductory theory needed in order to solve the problem. Thus, a student will open one of these worksheets and have a few pages of explanation of the problem, programming concepts employed in this activity, detail of the computational model (math equations), and an explanation of their meaning followed by sections of computer code with comments and instructions. Key sections of code will be removed from the solutions and this is what students will need to complete. The difficulty is designing these so that the student must incorporate some of the additional programming concepts they are learning while avoiding, as much as possible, the parts of the code that have concepts beyond their current understanding. The worksheet schedule will be as follows.

Personnel	Monday	Tuesday	Wednesday	Thursday	Friday
PI	Write problem and full solution	Write computational intro and remove sections of solution	Write modeling introduction with equations and figures/ illustrations	Work on JetStream setup* and template application	Adjust worksheet based on student feedback
Student	Re-solve the previous week's worksheet	Continue reading and studying relevant section of the textbook	Solving missing sections of the worksheet	Comment on intro, find online support material	Read and study relevant section of the textbook for next week

* described below

The student assistant and I will iterate through the process with the worksheet coding section being written by the PI, passed along to the student (who has spent time studying the material) in order to attempt and comment on what is unclear or does not work. This will then be refined and adjusted accordingly. At the same time the same will happen for the introduction section to ensure the worksheets are self-contained, including material the student found that was helpful to their learning. During this iterative process the PI will also work on the JetStream Virtual Machine (see below) setup and a template application for an education allocation on JetStream for any future instructor to use.

The JetStream Setup is a way to remove a significant difficulty of this class from the student experience. Students need to setup a computational environment that has the necessary software installed in order to work effectively with the python code and visualize the data. This is solved using a Virtual Machine (see both a non-expert and expert explanation).

Non-Expert Explanation: A Virtual Machine (VM) will appear to the student as a website they go and log onto in a web browser and see a Desktop environment (menu bar, icons to start programs etc.). When they full-screen their browser they will think they are on a regular computer desktop with all the tools they need already installed and working with icons ready. This is accomplished on a specialized supercomputer that will allow me to create a template for the system that students can easily access through the web portal. Thus, on day 1, they will have everything they need installed and working.

Expert Explanation: JetStream is a cluster that allows for creating custom VMs that can be launched, paused, check-pointed, and restarted (using different number of cpus, 1-44, and memory) through an XSEDE educational allocation. The VMs are access via a browser with a created XSEDE user id via internet 2 (now available at SIUE due to NSF award 1541435 PIs Chase, Cole and Ackad). The PI will create the VM from an empty Ubuntu VM image provided by JetStream (you must start from one of their images) with the anaconda python manager to give the students a VM with all the needed libraries (including visualizations) so that they have no software to install and there can be no issue with missing libraries. Each student will have their own copy of the VM which they can save their data, test and run their code. Additionally, jupyter-lab (and notebook) will be installed to give the student an easy to use IDE with easy visualization so the student can begin working immediately.

Thursday's work will thus include writing and refining a template JetStream application for the class to use JetStream for anyone who will teach the class in the future. Additionally, it will be used to modify the VM as new software needs are identified in the writing of the projects.

Qualifications of project directors to carry out the project: The PI has received numerous allocations on XSEDE including JetStream and has setup VMs for students before. The PI is also a trained Computational Physicists/Biophysicist with a minor in Computer Science. The undergraduate expected to participate is also a physics major with a computer science minor.

Alignment with EUE emphases: These projects are collaborative and fall under a high impact practice (HIP) as students will work in groups on challenging projects that will require team work as the subject matter may not be familiar to all students. For instance, in the Enzyme Kinetics project, chemistry and biology majors/minors will be able to help the other students with understanding the underlying science and its applicability as the team as a whole work together to finish the project.

c. **Evaluation**

This award will fund the creation of a new set of projects for a new physics course and thus there is no previous data to compare with. However, due to the fact that the projects are team based and have multiple parts it will be possible to perform a Longitudinal-Latitudinal project assessment. Each project has multiple pieces that the students will need to complete, using their newly acquired skills for more challenging tasks within the project. The grading will thus follow the group's latitudinal development through each assignment as well as longitudinally through each assignment (illustrated below).

Project	**Task 1**	**Task 2**	**Task 3**	**Task 4**	**...**
1					...
2					...
3					...
⋮	⋮	⋮	⋮	⋮	⋮

Evaluation will occur after the semester is finished. It is expected that the gradient of the scores for each group should be positive in all directions, meaning the students are getting better as they work through the projects (latitudinally) and as the semester goes on (longitudinally). Further statistical tools may be employed for more detailed analysis with the aid of Dr. Foster.

A negative slope in any direction will be an indication that a task was too simple (causing a local maximum) or too difficult and will be investigated to improve on for the next course iteration. Ultimately, success will be determined by having students enter subsequent courses and being able to use their new skills to solve, plot and visualize other course material or research projects they are engaged in.

Dissemination: The worksheets will be stored on the Physics Department shared drive for future instructors to access along with the template application material needed for the JetStream High Performance Computing award. This will allow anyone future instructor to teach and improve on the material created. Additionally, the JetStream Virtual Machine image will be made public so that anyone worldwide who wished to use the setup the PI has created can do so.

Budget and Budget Justification: Salaries ($3,468)

PI: The PI requests 1 month of summer salary at 100% effort ($7,116) to create the four projects. This is the time needed to create, test, and refine the needed projects as well as apply for the external supercomputing time and create the needed computing environment for the students in order to ensure the course is as accessible as possible. This will allow for the creation of four projects (about 1 per 4 weeks in the course it will be offered in).

Undergraduate Student: One month during the summer ($1,637) is requested for a student worker for 25 h/week at $15/hour in order to work with the PI and ensure the material is accessible, clear, and effective. Student pay rate is justified by the PI's experience with their previous Air Force grant and trying to recruit and retain students with a high degree of technical skills who would easy garner employment outside the university.

Other budget items: None

References

[1] Statement on Computational Physics (accessed Feb 18, 2019)

[2] AAPT Recommendations for Computational Physics in the Undergraduate Physics Curriculum (accessed Feb 19, 2019)

SIUE DEPARTMENT OF PHYSICS

TO: EUE EVALUATION COORDINATOR

FROM: PROFESSOR JACK GLASSMAN, CHAIR, DEPARTMENT OF PHYSICS

SUBJECT: SUPPORT FOR PROFESSOR ACKAD'S EUE PROPOSAL

DATE: MARCH 18, 2019

I have read the EUE proposal submitted by Professor Ackad entitled "Scaffolded Projects for Applied Numerical Science, Part of a new course in computational science for STEM students" and unequivocally support this proposal on behalf of the Department of Physics.

The traditional physics curriculum trains students in attacking physics problems as theoretical exercises or experimental problems. When doing traditional "theory," physicists develop mathematical models that yield functions which, in turn, can be used to predict laboratory or "real world" results. Since the 1980s (at least) computers have offered a "third way" of doing physics: rather than obtaining results by strictly performing mathematical operations, computer techniques of approximation and iteration. Numerical techniques are now absolutely core components in the toolbox of professional physicists. Yet undergraduate degree programs, such as the BS program offered by my department, rarely teach this crucial skill set. Our new course, PHYS219, will change that.

Professor Ackad is a highly productive member of my faculty and a world-class expert in the use of computational tools in physics. He has also demonstrated himself to be a talented teacher who has, since his arrival at SIUE in 2011, systematically studied physics pedagogy. His ability to implement well-considered pedagogic strategies into courses is well established. Since this course is at the heart of his scholarly expertise, I have very high hopes for its outcomes.

The proposed project will, if funded, allow Professor Ackad to develop a suite of tools that will maximize the early effectiveness of the course. These tools will be available to future instructors teaching the course, giving us an ongoing value for this upfront investment. Since the course is intended to teach students beyond solely physics majors, including students from a wide array of other STEM disciplines, the impact of this project will extend throughout the university. I know of no other course currently being offered at SIUE that teaches a similar set of skills, which corroborates the hope, expressed by Professor Ackad in his proposal, that the class will be populated by many non-physics majors. All of these students will gain very important, contemporary skills.

Without the funding requested in this proposal, Professor Ackad will not be able to develop the course tools needed for this class to be taught with maximum effectiveness. He will still teach the course, and I am confident that he will do a fine job. But the carefully-crafted procedures that he has laid out in the proposal will not be realizable unless he can spend the time needed to create them. The budget is modest, requesting only summer salary for himself and an undergraduate assistant. I think this small expenditure is a very worthwhile investment for the increase in course effectiveness that it promises to enable.

SOUTHERN ILLINOIS UNIVERSITY EDWARDSVILLE

COLLEGE OF ARTS AND SCIENCES, OFFICE OF THE DEAN

To: Excellence in Undergraduate Education

From: Greg Budzban, Dean, College of Arts and Sciences

Subject: Dean's Memo of Support

Date: 12 March, 2018

The College of Arts and Sciences strongly supports the application of Dr. Edward Ackad for an EUE grant to support development of course components for a newly proposed course, PHYS 219 - *Applied Numerical Science*. This course is intended to serve students in Physics as well as other majors dealing with computational models, as in Engineering. The integration of up-to-date applications is important to ensuring students are prepared professionally for use of industry standard techniques. As Dr. Ackad notes, the course focuses on providing students with practical programming skills applicable to a wide range of problems. Dr. Ackad's proposed course modules would allow for use of cloud-based programs and provide templates that could be used for other courses.

The majority of the budget is faculty salary to compensate effort in developing the course modules. Additional funds for student wages supports evaluation of the new exercises to ensure they will work as intended for the course. The project provides benefits beyond the project year, as the redesigned course components would continue to be used in future years.