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Federal Agency and Organization Element to Which Report is Submitted:	4900
Federal Grant or Other Identifying Number Assigned by Agency:	1547798
Project Title:	CREST: Center for Aquatic Chemistry and the Environment
PD/PI Name:	Todd A Crowl, Principal Investigator Shu-Ching Chen, Co-Principal Investigator Piero R Gardinali, Co-Principal Investigator Laird H Kramer, Co-Principal Investigator Rene M Price, Co-Principal Investigator
Recipient Organization:	Florida International University
Project/Grant Period:	04/15/2016 - 03/31/2021
Reporting Period:	04/15/2016 - 03/31/2017
Submitting Official (if other than PD\PI):	N/A
Submission Date:	N/A
Signature of Submitting Official (signature shall be submitted in accordance with agency specific instructions)	N/A

Accomplishments

* What are the major goals of the project?

1. Establish a functioning CREST Center, i.e., infrastructure, management, partners

2. Develop novel tools and solutions for the problem of water contamination across complex landscapes

3. Increase interest and participation by students from traditionally underrepresented groups in STEM research and careers

* What was accomplished under these goals (you must provide information for at least one of the 4 categories below)?

Major Activities:

Goal 1: Establish a functioning CREST Center, i.e., infrastructure, management, partners

Physical Infrastructure:

Because this is the first year of our CREST Center, much of our effort has been spent initiating the Center to maximize our success in terms of education, research and outreach. To that end, our major accomplishments include:

- Establishment of CREST Graduate student offices in both of our main campuses (MMC, BBC).
- Establishment of our Program Coordinator's Offices (associated with the grad offices above)
- Establishment of the CREST Student Analytic Lab facility
- Establishment of the CREST Research and Development Facility
- Establishment of the CREST Synthesis, Analysis and Visualization Facility

Human Infrastructure:

- Advertised for and hired a CREST Program Coordinator
- Advertised and hired two CREST Post-Doctoral Fellows (with other university funds)
- Appointed a Leadership team (see attached Organization Chart) that includes all colleges and departments currently participating in CREST

Program Management

- Appointed an External Advisory Board with Disciplinary, Education and CREST management expertise
- Established a network of External Partners to provide input into Research, Internship and Career pathways

Partnerships and Collaborations

- We held our first 'all-hands' meeting that formally established our partnerships with the external partners listed in participants
- Through our successful supplemental request, we have formalized a collaborating among FIU CREST, the University of Puerto Rico and the National Estuary Research Reserves in Florida and Puerto Rico
- Successfully submitted supplemental request for Mangrove research and expertise
- Successfully fostered a UPR CREST student's NSF CREST Post-Doctoral proposal to join the FIU CREST Program
- Successfully fostered a FIU CREST student's NSF CREST Post-Doctoral proposal to join the UNM CREST Program

Goal 2: Develop novel tools and solutions for the problem of water contamination across complex landscapes

Subproject 1: Stressor Detection

PhD student Paolo Benigni is studying the fundamental characteristics that define the conformational space of heteroatom polyaromatic hydrocarbons will be studied using IMS-FT-ICR MS and theoretical tools. In particular, new variants of IMS are being developed and coupled to ultrahigh resolution mass spectrometers for a more comprehensive characterization of complex mixtures.

PhD student Javier Rodriguez-Casariego is conducting epigenetic studies addressing the effects of pollutants and contaminants on model aquatic organisms; providing information about the impact of pollution on the health of these populations, the mechanisms participating in the onset of different levels of tolerance as well as development of epigenetic biomarkers of stress.

PhD student Cody Henderson is developing a comprehensive yet simple (field-deployable) isolation and pre-concentration protocol based on solid phase extraction, to produce extracts from environmental samples that could be analyzed directly by UPLC-HRMS (Orbitrap).

Subproject 2: Stressor Transport and Transformation

PhD student Ximena Mesa has started research on Wagner Creek, the largest tributary to the Miami River and most polluted waterbody in the State of Florida. Ximena is studying the effects of restoration (i.e., contaminated sediment removal and green infrastructure) on the ecosystem structure and function. Initial results indicate that water levels and dissolved oxygen concentrations in Wagner Creek are highly variable and often critically low.

Subproject 1 & 3: Stressor Detection and Data Analytics and Synthesis

The primary goal of this cross-Subproject research is to apply statistical analysis to two datasets; one contains the sampling information and the concentration of Total mercury (THg) and Methylmercury (MeHg) in water, soil, floc, periphyton, and mosquito fish; the other contains location information of each sampling site and the concentration of MeHg in Largemouth bass (LMB) and Sunfish. We hope to answer several questions: Are the years significantly different? If so, what are other parameters that make the significant changes? Moreover, are we able to say whether the data contains enough information to show the trend in mercury concentration through the years? With collaborative use of Subproject 3's data analysis tools, we have:

- Applied Cox-Stuart and Mann Kendall trend analysis to see if there is a significant change in the trends of concentration of THg and MeHg in water, soil, floc, periphyton, mosquito fish, LMB, and Sunfish.
- Applied the ANOVA test to evaluate if the changes in trend of concentration of THg and MeHg for different years is significant.
- Applied Tukey's method to assess the confidence interval for all the pairwise differences between the trends per year.

Subproject 2 & 3: Stressor Transport and Transformation and Data Analytics and

Synthesis

PhD student Kalli Unthank, is working with sub-project 3's PhD students on developing a Semantic Search on Hydrological Literature. Our goal is to develop a semantic search system for the environmental and hydrological research literature. This tool will make search of scholarly articles more precise for environmental domains, initially focusing on fate and transport of contaminants. The semantic search system will enable environmental and hydrological researchers to easily find relevant research papers. To date, they have:

- Designed a Natural Language Processing (NLP) pipeline for the semantic search system.
- Obtained around 11,000 academic papers published by Elsevier on the environmental domain. These papers will be indexed and searched by our system.
- Begun a pilot annotation study for identifying EnvO Environmental Ontology concepts in academic papers, thus developing gold-standard annotations to serve as ground truth to evaluate the performance of the semantic search system. We also wrote an annotation guide for standardizing how annotations are recorded.
- Deployed our system to environmental and hydrological researchers, to enhance their search through the academic literature.

Mangrove Supplement:

Planning meetings and conference calls took place in late 2016 and early 2017 among project participants, in south Florida and Puerto Rico, to establish priorities, choose coring locations, and plan field campaigns and student trips. A site scoping trip to Puerto Rico was conducted in February, 2017 to assess field logistics, meet with collaborators, and finalize coring locations. A collaboration was established with NASA to coordinate the collection of remotely-sensed data from Goddard's LiDAR, Hyperspectral and Thermal (G-LiHT) airborne imager at mangrove coring locations for March/April 2017. Field verification trips took place during those same months, with leaf spectral data collected for all mangrove species in each location. MOU's were (will be) signed between FIU and two National Esturarine Research Reserves (NERRs) – Rookery Bay NERR and Jobos Bay NERR. Cores were collected and vegetation sampled at a subset of south Florida locations.

Goal 3. Increase interest and participation by students from traditionally underrepresented groups in STEM research and careers

- Nine graduate students (4 Hispanic; 3 female) have been directly supported by CREST Stipends
- Three Post-Doctoral Fellows are participating in CREST (1 Hispanic; 3 female)

Specific Objectives: **Goal 3. Increase interest and participation by students from traditionally underrepresented groups in STEM research and careers**

- Recruited 16 PhD and 1 MS students as the first CREST Graduate Student cohort; 9 have been financially supported to-date
- Recruited three Postdoctoral Fellows as Affiliates of CREST to oversee the Analytic Teaching and Research Labs
- Designed a web site, flyers and other materials to advertise the CREST Center and the opportunities for student involvement

- We are currently recruiting external students for our second cohort
- Set up an informational booth for CREST recruitment at the 37th Annual meeting of the Society of Environmental Toxicology and Chemistry (SETAC) in Orlando, Nov. 2016.
- Co-sponsored an Environmental Cartoon Workshop with the Dutch Consulate, providing students with the tools to help them employ images and cartoons as a way of effectively spreading awareness of important environmental issues.
- Designed and developed the CREST CAChE Discovery 1 course on 'Research in Aquatic Ecosystems,' aimed at giving undergraduates first-hand experience with graduate-level research and introducing them to career pathways in STEM fields.
- Increased awareness and participation in the CREST Center through the BSC 5935 course, 'Philosophy of Science as a Means Towards Enhancing Interdisciplinary Research' currently taught by Prof. Crowl (Spring 2017).

Significant Results:

Goal 2. Develop novel tools and solutions for the problem of water contamination across complex landscapes

Subproject 1: Stressor Detection

Development of software package to validate the TIMS and FT-ICR MS instrumental performance, and build new processing tools for unsupervised characterization of complex mixtures; 'Software Assisted Molecular Elucidation' (SAME) can de-convolute TIMS-FT-ICR MS data, is currently applied to photo-irradiated water accommodated fractions of crude oils, and will be extended to analyze dissolved organic matter (DOM).

Significant decrease in global DNA methylation and modifications in DNA methylation patterns in indicator species during responses to aquatic toxins and nutrient stress. Increase in histone H2A.X phosphorylation levels in response to genotoxic stress caused by exposure to marine toxins and nutrient pollution in indicator species on coastal areas.

Development of an analytical method for the detection of common wastewater tracers (Caffeine, Splenda, Acetaminophen).

Subproject 1 & 3 Collaboration: Stressor Detection and Data Analytics and Synthesis

Cox-Stuart and Mann Kendall trend analysis were applied to the trends of total mercury in three different fishes. Based on multiple experiments, several trends were seen in the trends of MeHg in Largemouth bass (LMB), and Sunfish during the years (1999-2015) for different sampling sites.

ANOVA and Tukey test was applied to the trends of mercury (THg) concentration in mosquito fish for different latitudes grouped by the year the sample was collected. Students found out whether the change in the trend was significant and also whether the change in latitude and/or year had the most significant effect.

Subproject 2 & 3 Collaboration: Stressor Transport and Transformation and Data Analytics and Synthesis

Students identified state of the art semantic search systems, in particular, BabelNet, Mimir (Multiparadigm Indexing and Retrieval), and Semantic Scholar. These systems are endowed with domain specific knowledge through use of ontologies. To give the

semantic search knowledge about the environmental domain the collaborating students will use the EnvO Environmental Ontology. It will be used for the concept disambiguation in the semantic search pipeline. Scholarly articles will be indexed using the concepts in EnvO and queries will have concepts extracted from them. The concepts embedded in the queries and literature texts will be used in the semantic search pipeline.

Key outcomes or Other achievements:	**Goal 2. Develop novel tools and solutions for the problem of water contamination across complex landscapes**

Subproject 1:

- Established baseline data on epigenetic responses of different aquatic organisms during exposure to different sources of pollution, natural and anthropogenic.

Subproject 1 & 3 Collaboration:

- For most of the statistical tests, we applied we used R, which is a language and environment built primarily for manipulating data, performing calculations and building graphical representations of data.
- We identified a lot of statistical and graphical techniques within R.

Subproject 2 & 3 Collaboration:

- Identified the techniques that state of the art semantic search use
- Incorporated these approaches into the design of our system.
- Ran a pilot annotation study of EnvO concepts in the scientific literature.
- Wrote an annotation guide for annotating EnvO concepts.
- Designed a prototype semantic search system.

* What opportunities for training and professional development has the project provided?

Education:

We designed and are currently offering a graduate course (BSC 5935-U02), entitled 'Philosophy of Science as a Means Towards Enhancing Interdisciplinary Research' (Syllabus attached).

We have been designing the CREST Discovery Course. Two sections, each planned for 25 students, are scheduled to be offered in Fall 2017.

Objectives:

- Bring students together from all interests and career paths, and challenge them to "do science" and think like scientists
- Give students hands-on experience with locally-relevant data and raise awareness of environmental issues impacting South Florida

Learning Outcomes:

- Experience authentic, graduate-level environmental research
- Formulate testable hypotheses, design procedures and experiments to test hypotheses and draw conclusions
- Gain knowledge regarding the environmental issues currently impacting local South Florida aquatic ecosystems
- Efficiently communicate research findings to classmates and local stakeholders through poster presentations

<u>Subproject 1 & 3 Collaboration</u>:

- We had the opportunity to afford cross-disciplinary work between people from Chemistry and Computer Science.
- Apply different types of statistical analysis to a data set and make conclusions according to the result.
- Establish weekly meetings where we communicate the progress and what are the next steps.

<u>Subproject 2 & 3 Collaboration</u>:

- We have been working closely with CREST CAChE domain experts from the hydrology. This has allowed us to figure out how the group members with natural language processing and computer science background can help expedite the research of the hydrologists.
- We are beginning an annotation study where we will hire and train undergraduates in the environmental domain to annotate scholarly papers for EnvO Environmental Ontology concepts. This will involve more students in the interdisciplinary effort.

* How have the results been disseminated to communities of interest?

<u>Subproject 1</u>:

Participant Paolo Benigni received CREST support to travel and present his work titled "Towards structural molecular analysis of complex samples using TIMS-FT-ICR MS" at the Emerging Researchers National conference in Washington D.C. This presentation focused on the CREST Center's goal of improving the ability to sense pollutants by using novel instrumental techniques such as TIMS-FT-ICR MS.

<u>Subproject 1 & 3</u>:

We have engaged in cross-disciplinary dissemination within the subgroup.

<u>Subproject 2 & 3</u>:

Our findings about state of the art semantic search systems, and how they influenced the system we are building, have been shared within the CREST center at FIU.

* What do you plan to do during the next reporting period to accomplish the goals?

<u>Center-wide</u>:

We will act on the feedback provided by CREST CAChE's External Advisory Committee (EAC); see attached PDF file that the EAC presented at the conclusion of our All-hands meeting held March 9-10, 2017.

<u>Subproject 1 & 3 Collaboration</u>:

For the next reporting period, we plan to build a theoretical model to show the structural relationships between the variables in the dataset. Then, we want to apply Structural Equation Model (SEM) to see if the model fits the dataset.

<u>Subproject 2 & 3 Collaboration</u>:

Build a prototype semantic search system for the environmental and hydrological domains.

Evaluate the performance of the semantic search system.

Extend the EnvO Environmental Ontology to contain topics more relevant to the Everglades and contaminants.

Conduct an annotation study to produce gold-standard annotations for evaluation of the performance of the semantic search

system.

Deploy the system to hydrological and environmental researchers, and get their feedback on the effectiveness of the system.

<u>Mangrove Supplement:</u>

Meeting between collaborators will take place in San Juan, Puerto Rico in June 2017

Cores will be collected and dated using 210Pb for determination of sediment accretion rates at each site; aboveground biomass will be estimated at each site

Student exchange between UPR and FIU students will take place in June 2017 with students traveling to sites in both south Florida and Puerto Rico. Students will learn about sample preparation, data collection, data analysis, environmental conditions and hydrologic regimes for mangrove forests in each region.

Project goals and preliminary data will be presented by students, post-docs, and PIs at the Society of Wetland Science Meeting in San Juan, PR in Jun 6-8, 2017

NASA G-LiHT data will be obtained and analyzed to determine canopy heights, plant stress, and species composition at associated coring locations in PR and south Florida

Supporting Files

Filename	Description	Uploaded By	Uploaded On
CREST_CAChE_Org_Chart_March-2017.pdf	CREST CAChE Organizational Chart	Todd Crowl	03/20/2017
FIU CREST CAChE External Advisory Committee Feedback March 2017.pdf	CREST CAChE EAC Feedback March 2017	Todd Crowl	03/20/2017
BSC-5935-Syllabus_Spring-2017.pdf	Syllabus for CREST CAChE-designed course, Philosophy of Science as a Means Towards Enhancing Interdisciplinary Research	Todd Crowl	03/20/2017

Products

Books

Book Chapters

Inventions

Journals or Juried Conference Papers
Haiman Tian and Shu-Ching Chen (2017). MCA-NN: Multiple Correspondence Analysis based Neural Network for Disaster Information Detection. *The Third IEEE International Conference on Multimedia Big Data (IEEE BigMM 2017)*. . Status = ACCEPTED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

Hilary Flower, Mark Rains, David Lewis, Jia-Zhong Zhang, René Price (2017). Saltwater intrusion as potential driver of

phosphorus release from limestone bedrock in a coastal aquifer. *Estuarine, Coastal and Shelf Science*. 184 166. Status = PUBLISHED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes ; DOI: 10.1016/j.ecss.2016.11.013

Rodrigo Gonzalez-Romero, Victoria Suarez-Ulloa, Javier Rodriguez-Casariego, Daniel Garcia-Souto, Gabriel Diaz, Abraham Smith, Juan Jose Pasantes, Gary Rand, Jose M. Eirin-Lopez (2017). Effects of Florida Red Tides on histone variant expression and DNA methylation in the Eastern oyster Crassostrea virginica. *Aquatic Toxicology*.   . Status = AWAITING_PUBLICATION; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes ; DOI: 10.1016/j.aquatox.2017.03.006

Samira Pouyanfar and Shu-Ching Chen (2017). T-LRA: Trend-based Learning Rate Annealing for Deep Neural Network. *The Third IEEE International Conference on Multimedia Big Data (IEEE BigMM 2017)*.   . Status = ACCEPTED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

Licenses

Other Conference Presentations / Papers

Javier Rodriguez-Casariego, Sean Campbell, Mark Ladd, Andrew Shantz, Steven Roberts, Deron Burkepile, Jose Eirin-Lopez (2016). *Preliminary analysis of the epigenetic mechanisms underlying acclimatory responses to nutrient pollution in stony corals*. 7th SETAC (Society of Environmental Toxicology and Chemistry) World Congress / SETAC North America 37th Annual Meeting. Orlando, FL. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Paolo Benigni, Mark E. Ridgeway, Melvin A. Park, and Francisco Fernandez-Lima (2017). *Towards structural molecular analysis of complex samples using TIMS-FT- ICR MS*. Emerging Researchers National (ERN) Conference in Science, Technology, Engineering and Mathematics (STEM). Washington, DC. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Other Products
Databases.

Subprojects 2 & 3 are creating annotations of hydrology academic papers for concepts from the ENVO environmental ontology.

Other Publications

Patents

Technologies or Techniques

Subprojects 2 & 3 are developing a semantic search system on hydrological and environmental academic papers.

Thesis/Dissertations

Websites
CREST CAChE Website
http://crestcache.fiu.edu

This is the Center's website. Content and format are still being being added and update processes are being established.

Participants/Organizations

What individuals have worked on the project?

Name	Most Senior Project Role	Nearest Person Month Worked
Crowl, Todd	PD/PI	0
Chen, Shu-Ching	Co PD/PI	0
Gardinali, Piero	Co PD/PI	0
Kramer, Laird	Co PD/PI	0
Price, Rene	Co PD/PI	0
Anderson, Bill	Faculty	0
Cai, Yong	Faculty	0
Cooke, Marcus	Faculty	0
Eirin-Lopez, Jose	Faculty	0
Felty, Quentin	Faculty	0
Fernandez Lima, Francisco	Faculty	0
Finlayson, Mark	Faculty	0
Fourqurean, James	Faculty	0
Gaiser, Evelyn	Faculty	0
Heithaus, Michael	Faculty	0
Jaffe, Rudolf	Faculty	0
Kominoski, John	Faculty	0
Li, Tao	Faculty	0
Meeder, John	Faculty	0
Melesse, Assefa	Faculty	0
Rand, Gary	Faculty	0

Ross, Michael	Faculty	0
Scionto, Leonard	Faculty	0
Vassigh, Shahin	Faculty	0
Ding, Yan	Postdoctoral (scholar, fellow or other postdoctoral position)	0
Ogurcak, Danielle	Postdoctoral (scholar, fellow or other postdoctoral position)	0
Rodriguez, Carmen	Postdoctoral (scholar, fellow or other postdoctoral position)	0
Dominguez, Dolores	Other Professional	1
Graham, Scott	Other Professional	1
Schonhoff, Bradley	Other Professional	6
Teutonico, Rita	Other Professional	1
Kershaw, Mark	Technician	1
Banisakher, Deya	Graduate Student (research assistant)	6
Benigni, Paolo	Graduate Student (research assistant)	6
Eisenberg, Joshua	Graduate Student (research assistant)	2
Mesa, Ximena	Graduate Student (research assistant)	6
Regier, Peter	Graduate Student (research assistant)	6
Rodriguez Casariego, Javier	Graduate Student (research assistant)	6
Smith, Abraham	Graduate Student (research assistant)	2
Unthank, Kalli	Graduate Student (research assistant)	6
Yanez Zapata, Tiffany	Graduate Student (research assistant)	3

Full details of individuals who have worked on the project:

Todd A Crowl
Email: tcrowl@fiu.edu
Most Senior Project Role: PD/PI
Nearest Person Month Worked: 0

Contribution to the Project: Center Director Supervised Graduate Assistant Tiffany Yanez Zapata

Funding Support: FIU

International Collaboration: No
International Travel: No

Shu-Ching Chen
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Most Senior Project Role: Co PD/PI
Nearest Person Month Worked: 0

Contribution to the Project: Co-leader, Subproject 3

Funding Support: FIU

International Collaboration: No
International Travel: No

Piero R Gardinali
Email: gardinal@fiu.edu
Most Senior Project Role: Co PD/PI
Nearest Person Month Worked: 0

Contribution to the Project: Associate Director, Research and Facilities Co-leader, Subproject 1

Funding Support: FIU

International Collaboration: No
International Travel: No

Laird H Kramer
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Most Senior Project Role: Co PD/PI
Nearest Person Month Worked: 0

Contribution to the Project: Leader of Center's Educational Initiatives as Director of FIU's STEM Transformation
Institute

Funding Support: FIU

International Collaboration: No
International Travel: No

Rene M Price
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Most Senior Project Role: Co PD/PI
Nearest Person Month Worked: 0

Contribution to the Project: Co-leader, Subproject 2 Supervised Graduate Assistant Kalli Unthank

Funding Support: FIU

International Collaboration: No
International Travel: No

Bill Anderson
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subproject 1

Funding Support: FIU

International Collaboration: No
International Travel: No

Yong Cai
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Co-lead, Subproject 1

Funding Support: FIU

International Collaboration: No
International Travel: No

Marcus Cooke
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Co-lead, Subproject 3

Funding Support: FIU

International Collaboration: No
International Travel: No

Jose M Eirin-Lopez
Email: jeirinlo@fiu.edu
Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subprojects 1 & 3, Supervised Graduate Assistant Javier A. Rodriguez Casariego

Funding Support: FIU

International Collaboration: No
International Travel: No

Quentin Felty
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subprojects 1 & 3

Funding Support: FIU

International Collaboration: No
International Travel: No

Francisco A Fernandez Lima
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subprojects 1 & 2, Supervised Graduate Assistant Paolo Benigni

Funding Support: FIU

International Collaboration: No
International Travel: No

Mark A Finlayson
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subproject 3; Supervised Graduate Assistants Deya Banisakher and Joshua Eisenberg

Funding Support: FIU

International Collaboration: No

International Travel: No

James Fourqurean
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subproject 2

Funding Support: FIU

International Collaboration: No
International Travel: No

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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subproject 2

Funding Support: FIU

International Collaboration: No
International Travel: No

Michael Heithaus
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subproject 1&3; Supervised Graduate Assistant Abraham Smith

Funding Support: FIU

International Collaboration: No
International Travel: No

Rudolf Jaffe
Email: jaffer@fiu.edu
Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Co-lead, Subproject 2 Supervised Graduate Assistant Peter Regier

Funding Support: FIU

International Collaboration: No

International Travel: No

John Kominoski
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subproject 2; Supervised Graduate Assistant Ximena Mesa

Funding Support: FIU

International Collaboration: No
International Travel: No

Tao Li
Email: taoli@cs.fiu.edu
Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subproject 3

Funding Support: FIU

International Collaboration: No
International Travel: No

John F Meeder
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Mangrove Supplement

Funding Support: FIU

International Collaboration: No
International Travel: No

Assefa Melesse
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subproject 2

Funding Support: FIU

International Collaboration: No

International Travel: No

Gary Rand
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subproject 3

Funding Support: FIU

International Collaboration: No
International Travel: No

Michael Ross
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Mangrove Supplement

Funding Support: FIU

International Collaboration: No
International Travel: No

Leonard Scionto
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Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Suprojects 1 & 2

Funding Support: FIU

International Collaboration: No
International Travel: No

Shahin Vassigh
Email: svassigh@fiu.edu
Most Senior Project Role: Faculty
Nearest Person Month Worked: 0

Contribution to the Project: Participated in Subproject 3

Funding Support: FIU

International Collaboration: No

International Travel: No

Yan Ding
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Most Senior Project Role: Postdoctoral (scholar, fellow or other postdoctoral position)
Nearest Person Month Worked: 0

Contribution to the Project: Participating in CREST research

Funding Support: FIU

International Collaboration: No
International Travel: No

Danielle Ogurcak
Email: dogurcak@fiu.edu
Most Senior Project Role: Postdoctoral (scholar, fellow or other postdoctoral position)
Nearest Person Month Worked: 0

Contribution to the Project: Participating in CREST research

Funding Support: FIU

International Collaboration: No
International Travel: No

Carmen Rodriguez
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Most Senior Project Role: Postdoctoral (scholar, fellow or other postdoctoral position)
Nearest Person Month Worked: 0

Contribution to the Project: Participating in CREST research

Funding Support: FIU

International Collaboration: No
International Travel: No

Dolores Dominguez
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Most Senior Project Role: Other Professional
Nearest Person Month Worked: 1

Contribution to the Project: clerical support to the project

Funding Support: none

International Collaboration: No

International Travel: No

Scott Graham
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Most Senior Project Role: Other Professional
Nearest Person Month Worked: 1

Contribution to the Project: Associate Director, Coordination and Strategy

Funding Support: FIU

International Collaboration: No
International Travel: No

Bradley Schonhoff
Email: bschonho@fiu.edu
Most Senior Project Role: Other Professional
Nearest Person Month Worked: 6

Contribution to the Project: Program Coordinator

Funding Support: none

International Collaboration: No
International Travel: No

Rita Teutonico
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Most Senior Project Role: Other Professional
Nearest Person Month Worked: 1

Contribution to the Project: Associate Director, Education and Training

Funding Support: FIU

International Collaboration: No
International Travel: No

Mark D Kershaw
Email: kershawm@fiu.edu
Most Senior Project Role: Technician
Nearest Person Month Worked: 1

Contribution to the Project: technical support for CREST facilities

Funding Support: none

International Collaboration: No

International Travel: No

Deya M Banisakher
Email: dbani001@fiu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: Participated in Subproject 3 under the supervision of Prof. Finlayson

Funding Support: None

International Collaboration: No
International Travel: No

Paolo Benigni
Email: pbenigni@gmail.com
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: Participated in Subproject 1 under the supervision of Prof. Fernandez-Lima

Funding Support: None

International Collaboration: No
International Travel: No

Joshua D Eisenberg
Email: jeise003@fiu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 2

Contribution to the Project: Participated in Subproject 3 under the supervision of Prof. Finlayson

Funding Support: None

International Collaboration: No
International Travel: No

Ximena Mesa
Email: xmesa002@fiu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: Participated in Subproject 2 under the supervision of Prof. Kominoski

Funding Support: None

International Collaboration: No

International Travel: No

Peter Regier
Email: pregi002@fiu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: Participated in Subproject 2 under the supervision of Prof. Jaffe; accepted CREST Postdoctoral Research Fellowship (PRF) to UNM CREST starting in Fall 2017 after his anticipated graduation in Summer 2017

Funding Support: None

International Collaboration: No
International Travel: No

Javier A Rodriguez Casariego
Email: javirodr@fiu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: Participated in Subproject 1 under the supervision of Prof. Eirin-Lopez

Funding Support: None

International Collaboration: No
International Travel: No

Abraham J Smith
Email: asmit065@fiu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 2

Contribution to the Project: Participated in Subproject 3 under the supervision of Prof. Heithaus

Funding Support: None

International Collaboration: No
International Travel: No

Kalli G Unthank
Email: kunth001@fiu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 6

Contribution to the Project: Participated in Subproject 2 under the supervision of Prof. Price

Funding Support: None

International Collaboration: No
International Travel: No

Tiffany N Yanez Zapata
Email: tyane001@fiu.edu
Most Senior Project Role: Graduate Student (research assistant)
Nearest Person Month Worked: 3

Contribution to the Project: Participated in the Education Thrust under the supervision of Prof. Crowl

Funding Support: FIU

International Collaboration: No
International Travel: No

What other organizations have been involved as partners?

Name	Type of Partner Organization	Location
Jobos Bay National Estuarine Research Reserve	State or Local Government	Aguirre, PR
Rookery Bay National Estuarine Research Reserve	State or Local Government	Naples, FL
University of Puerto Rico	Academic Institution	Rio Piedras, PR
University of South Florida	Academic Institution	Tampa, FL

Full details of organizations that have been involved as partners:

Jobos Bay National Estuarine Research Reserve

Organization Type: State or Local Government
Organization Location: Aguirre, PR

Partner's Contribution to the Project:
Facilities

More Detail on Partner and Contribution: Collaborating as an observation site for the Mangrove supplement

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Rookery Bay National Estuarine Research Reserve

Organization Type: State or Local Government
Organization Location: Naples, FL

Partner's Contribution to the Project:
Facilities

More Detail on Partner and Contribution: Collaborating as an observation site for the Mangrove supplement

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University of Puerto Rico

Organization Type: Academic Institution
Organization Location: Rio Piedras, PR

Partner's Contribution to the Project:
Facilities
Collaborative Research
Personnel Exchanges

More Detail on Partner and Contribution: Working with Jess Zimmerman, Professor, UPR, Program Director Luquillo LTER and El Verde Field Station Scientific Director and Alonso Ramirez, Associate Professor, UPR, as partners in the Mangrove supplement

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University of South Florida

Organization Type: Academic Institution
Organization Location: Tampa, FL

Partner's Contribution to the Project:
Facilities
Collaborative Research
Personnel Exchanges

More Detail on Partner and Contribution: Working with Donny Smoak, Professor, USF, will use radionuclides as tracers to establish sediment accretion rates in mangrove soils

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What other collaborators or contacts have been involved?
Nothing to report

Impacts

What is the impact on the development of the principal discipline(s) of the project?

Subproject 2 & 3 Collaboration:

The collaborative project will enrich both the fields of computer science and environmental science in the following ways:

- Computer Science: The system to be developed will serve as the state-of-the-art for ontology-based semantic search
- Environmental Science: The system to be developed will yield better literature-search results necessary to the environmental science community. The project will also engage young researchers in Environmental Science in cutting-edge information technology, increasing technical depth in this area as well as the chance of cross-disciplinary collaborations in the future

<u>Subproject 1 & 3 Collaboration</u>:

- Environmental Science: The collaborative project will enrich the field of environmental science by introducing more complex analytical approaches to environmental datasets. The results from data analysis can help us draw conclusions about what approaches could be taken to reduce the concentration of mercury. A documentation of different approaches for data analysis can also help other researchers apply the same analysis and observe the results for a different dataset.
- Computer Science: The applied methods will be helpful to find patterns and trends in different datasets. These statistical tests can also be helpful to evaluate the significance of different algorithms in computer science.

<u>Mangrove Supplement</u>:

- The project has already had positive impacts through the creation of partnerships with estuarine research reserves to assess valuable mangrove ecosystems. This partnership is mutually beneficial as students will gain experience from working in coastal environment and in labs located within the reserves, while NERRs will receive needed field and lab assistance to assess natural resources.

What is the impact on other disciplines?

<u>Subproject 2 & 3 and Subproject 1 & 3 Collaborations</u>:

The systems to be developed can be applied to other disciplines given the data necessary: as ontologies and knowledge bases develop for other fields such as astrology, biology, medical sciences, political sciences and humanities, the methods to be carried in this project can be implemented for those fields (and much more).

What is the impact on the development of human resources?

This project will help promote cross-disciplinary research to students from other fields. It will also help hone the students' academic and professional skills including – but not limited to – research method planning and development, research-specific critical thinking, exposure to interdisciplinary communication and collaboration, professional circle build-up, proposal and report preparation etc.

FIU PhD graduate Peter Regier has accepted a CREST Postdoctoral Research Fellowship and will be working under the guidance of Dr. Ricardo Gonzalez-Pinzon, in conjunction with the CREST Center for Water and the Environment at the University of New Mexico, to understand the effects of dissolved organic matter composition on nutrient spiraling dynamics along the Rio Grande river network. This project combines ongoing research involving high-frequency in situ water quality information and nutrient uptake experiments with his interests in organic matter quality as a driver of aquatic ecosystems along complex gradients of natural, urban and agricultural land use. The team's combined approach to collecting this wide array of datasets across a broad spatiotemporal spectrum will provide an unprecedented level of understanding of nutrient cycling along an arid-land river continuum. Through their research, they will seek to deliver valuable tools for monitoring aquatic ecosystems and aid in closing water and nutrient loops in resource-depleted systems.

What is the impact on physical resources that form infrastructure?

Because this is the first year of our CREST Center, much of our effort has been spent initiating the Center to maximize our success in terms of education, research and outreach. To that end, our major accomplishments include:

- Establishment of CREST Graduate student offices in both of our main campuses (MMC, BBC).
- Establishment of our Program Coordinator's Offices (associated with the grad offices above)
- Establishment of the CREST Research and Development Facility
- Establishment of the CREST Synthesis, Analysis and Visualization Facility
- Established the CAChE Nutrient Analysis Core Lab, which provides three distinct services and opportunities in separated spaces; a NELAC accredited nutrient analyses laboratory providing support for research and operated as a recharge

facility; a dedicated student training area for traditional water quality analyses; and a new technology improvement laboratory to provide support to develop alternative or novel techniques using liquid chromatography (LC), gas chromatography (GC) and ion Chromatography (IC).

This recharge facility provides NELAC-certified analyses of dissolved and total nutrients, dissolved organic carbon (DOC), total organic carbon (TOC), chlorophyll-a in fresh/salt waters, and total P in solids and tissue samples. Additional, non-certified analyses include total N and C, salinity, pH, dissolved oxygen, temperature, turbidity, etc. The CAChE Nutrient Analysis Core Lab currently serves FIU faculty and federal and government agencies, such as Monroe and Broward County, SFWMD, FDEPA, USEPA, etc. Its core equipment includes spectrophotometers, nutrient analyzers, C/N elemental analyzers, total N analyzers, TOC analyzers, ultrafiltration units, scintillation counters, etc.

The student teaching/development branch of the CAChE Lab allows students and post-doctoral associates to get hands-on experience with traditional chemical analysis, and explore advanced analytical instrumentation by introducing new techniques in support of their own research for environmental studies or professional development purposes. Examples of equipment and capabilities include:

- GC coupled with FID/ECD/TCD detectors for the analyses of common and greenhouse gases.
- HPLC-PDS for pigment separation and analysis
- IC to detect anions and cations in surface waters and wastewaters
- Nanodrop Scanning Spectrofluorometer for the measurement of fluorescent organic matter (FOM), algal pigments and environmental tracers.
- UV-Vis spectrophotometer for colorimetric water quality and measurements of optical properties for natural waters.

What is the impact on institutional resources that form infrastructure?

Human Infrastructure:

- Advertised for and hired a CREST Program Coordinator
- Advertised and hired three CREST-affiliated Post-Doctoral Fellows (with other university funds)
- Appointed a Leadership team that includes all colleges and departments currently participating in CREST

What is the impact on information resources that form infrastructure?

Data set on literature of the fate and transport of mercury and sulfur in the environment is being collected.

A well-structured environmental ontology will be developed using existing sparse ontologies. Thus, adding and enriching the environmental information resources and infrastructure.

We purchased two types of software for Ph.D. student projects: a type of keylogging/user interaction software to track literature search methods as well as two ARC GIS licenses for student research use.

What is the impact on technology transfer?

The literature search system being developed will increase the efficiency and efficacy of literature search performed by environmental researchers, decision makers, and the larger community. This will allow for a more agile and targeted technology transfer.

What is the impact on society beyond science and technology?

Subproject 2 & 3 Collaboration:

The overall project will result in the development of a data warehouse for water and environmental contamination in south Florida which will aid decision makers and policy enforcers in planning and managing environmental resources.

<u>Subproject 1 & 3 Collaboration</u>:

The overall system can help us determine different approaches that can be taken in order to reduce the concentration of mercury but determined what variables have the most impact in the changes for the trend.

Changes/Problems

Changes in approach and reason for change
Nothing to report.

Actual or Anticipated problems or delays and actions or plans to resolve them
Nothing to report.

Changes that have a significant impact on expenditures
Nothing to report.

Significant changes in use or care of human subjects
Nothing to report.

Significant changes in use or care of vertebrate animals
Nothing to report.

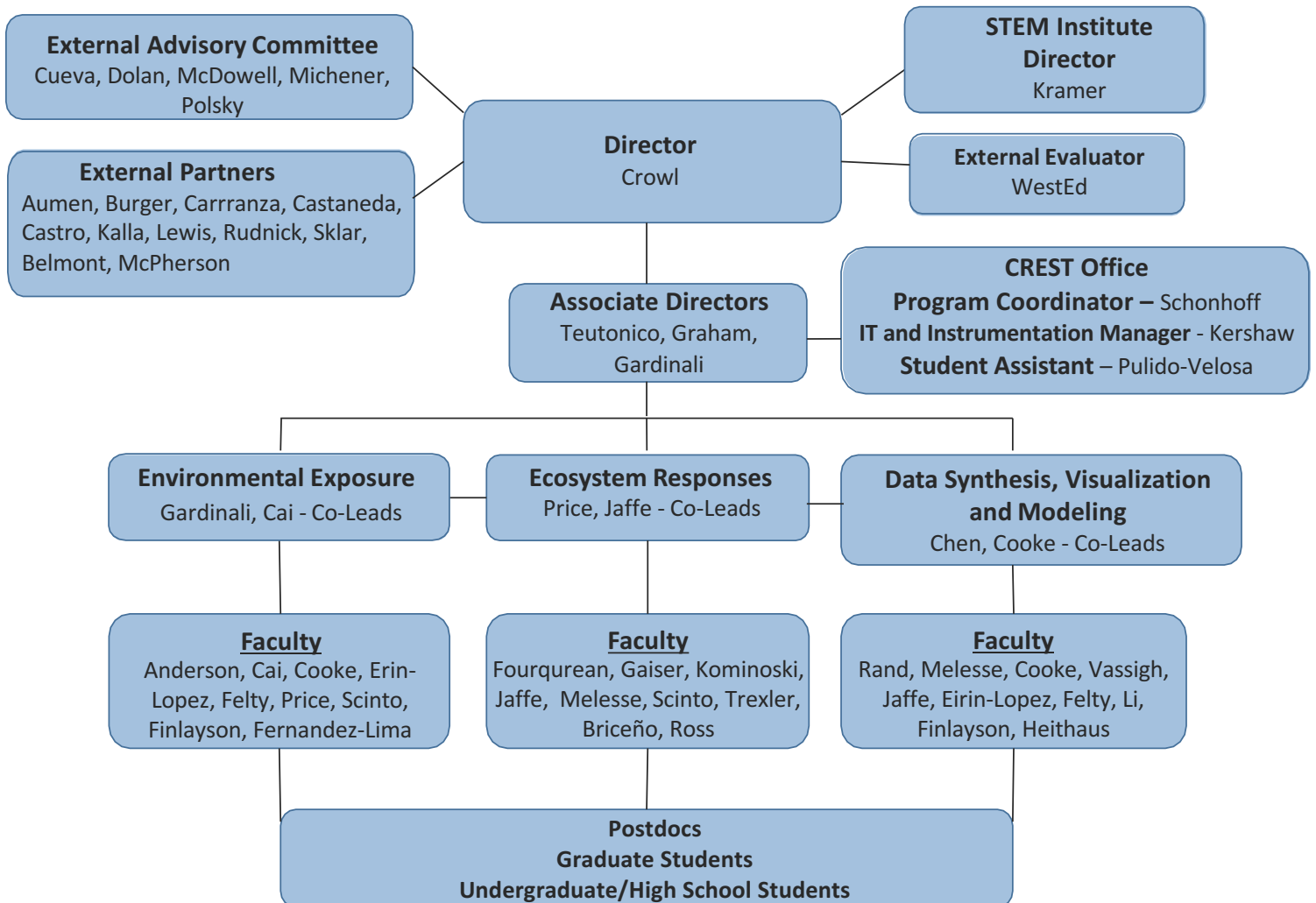**Significant changes in use or care of biohazards**
Nothing to report.

Organizational Structure

External Advisory Committee
Cueva, Dolan, McDowell, Michener, Polsky

External Partners
Aumen, Burger, Carrranza, Castaneda, Castro, Kalla, Lewis, Rudnick, Sklar, Belmont, McPherson

STEM Institute Director
Kramer

Director
Crowl

External Evaluator
WestEd

Associate Directors
Teutonico, Graham, Gardinali

CREST Office
Program Coordinator – Schonhoff
IT and Instrumentation Manager - Kershaw
Student Assistant – Pulido-Velosa

Environmental Exposure
Gardinali, Cai - Co-Leads

Ecosystem Responses
Price, Jaffe - Co-Leads

Data Synthesis, Visualization and Modeling
Chen, Cooke - Co-Leads

Faculty
Anderson, Cai, Cooke, Erin-Lopez, Felty, Price, Scinto, Finlayson, Fernandez-Lima

Faculty
Fourqurean, Gaiser, Kominoski, Jaffe, Melesse, Scinto, Trexler, Briceño, Ross

Faculty
Rand, Melesse, Cooke, Vassigh, Jaffe, Eirin-Lopez, Felty, Li, Finlayson, Heithaus

Postdocs
Graduate Students
Undergraduate/High School Students

Florida International University

CREST Center for Aquatic Chemistry and Environment

External Advisory Board Report March 2017

EAB Members

Erin Dolan eldolan@uga.edu, University of Georgia

William Michener william.michener@gmail.com, University of New Mexico

William H. McDowell bill.mcdowell@unh.edu University of New Hampshire

OVERVIEW – Center for Aquatic Chemistry and the Environment

This CREST project supports training of undergraduate, graduate, and post-doctoral students in STEM fields in a wide range of disciples. The project is well-conceived, focusing on three thematic areas (Environmental Exposure, Ecosystem Response, and Modeling). Each of the themes is addressed at multiple sites, which are readily accessible to project participants through the strong infrastructure provided by Southeastern Environmental Research Center (SERC). The core emphasis on the Everglades, the defining natural feature of south Florida, is appropriate and resonates with participants. The expansion through a supplement that focuses on mangroves in collaboration with another CREST project at the University of Puerto Rico is an excellent addition to the project as originally written due to the strong physical interconnections between the Everglades complex and coastal systems.

The project is off to an excellent start. The faculty are actively engaged in bridging across disciplines, recruiting students, and developing entry points into the CREST project that are consistent across administrative units and highly visible to potential participants. By building around a cohort of existing students whose work and intellectual interests are of direct relevance to CAChE, a nucleus of engaged and effective students has already been created within the first few months of funding. Interactions of the EAB with these students during the All Hands Meeting and at their posters shows that they are engaged, excited, and conducting high-quality work in their individual research projects. Support from FIU administration has been outstanding, with hiring of two post-docs and payment of tuition for graduate student participants being two particularly noteworthy contributions that will enhance the project's overall effectiveness and impact. The number of external partners is extraordinary, and among them they highlight the wide range of STEM employment opportunities that are found in the local community.

OPPORTUNITIES AND CHALLENGES

The following more specific observations and recommendations highlight our input to the project beyond what was presented at the All Hands meeting (see attached five-slide Powerpoint).

1. Maintain consistent names and messaging for the three focal areas. For example, area 1, often described as "Detection and identification," is also called "Environmental Exposure" as well as given other, even longer titles. Long descriptive titles are not helpful, as they have little meaning to those from other disciplines and likely undermine project participants' ability to develop a sense of the big picture. Consider developing a pictorial representation or concept map of the whole project (research themes, training activities, stakeholders) that can serve as a reference for all project personnel and participants to see where they "fit" and how the project elements inter-relate.

2. Develop simple and easily communicated assessments of annual progress toward explicit objectives. A traffic light system (green, yellow, red) would provide the needed level of detail and would provide a quick overview of progress toward major objectives.

3. The external partners are a very diverse group with different (but potentially conflicting) perspectives and priorities. The leadership team should devise an explicit strategy for interacting with their partners in a way that maximizes benefits to students and all stakeholders.

Establishment of a simple but clearly articulated process for developing these interactions with external partners and tracking their outcomes would be desirable.

4. Development of a Discovery course that serves to engage a broad cohort of FIU students is an excellent idea. Success of the course will depend on continued effort and input from faculty across multiple disciplines and academic units. Clear articulation of the overarching goals in offering such a course will enhance its likelihood of success.

5. Use of external evaluators to assess the effectiveness of CAChE in meeting educational objectives is commendable. The faculty should work closely with the evaluators to ensure that a rigorous evaluation can be conducted that is not overly dependent on meeting enrollment projections in the Discovery course, as it is difficult to predict enrollment for new courses. The idea of involving DBER faculty members in aspects of the evaluation or in studying project activities is intriguing, but would need to be carefully planned in order to avoid placing undue pressure on junior colleagues and to ensure data are collected and analyses are conducted in a way that is publishable.

6. The first All Hands meeting focused primarily on the research themes and research progress. Given the training nature of the project, it is important to identify training themes, clearly articulate training goals and objectives at all levels (undergraduate, graduate, post-doctoral) with respect to the themes, and align project activities with these goals and objectives. This process will help with stakeholder buy-in to the training elements of the project (e.g., internships with external partners) and with other aspects of project decision-making such as when and how to build trainees' awareness of diverse career paths, when and how to further trainees' communication skills (e.g., learning to give two-minute elevator speeches), and whether and how an additional EAB member could help to improve training.

<u>Philosophy of Science as a Means Towards Enhancing Interdisciplinary Research.</u>
<u>BSC 5935 U02</u>
<u>OE-112, Wednesday 3-5 and other arranged times</u>
<u>Prof. Todd A. Crowl</u>
<u>Spring 2017</u>

In this seminar, we will explore the ways that biological and physical scientists as well as engineers and computer scientists approach scientific understanding. The course is designed as a discussion seminar in which graduate and senior undergraduate students will be introduced to a brief history of the philosophy of science and the underlying importance of logic resulting in how we design, carry out and use mathematics and statistics to understand the world around us.

After the first couple of introductory discussion that I will lead, we will have students lead discussions of the chapters or papers for that week's discussion. Our only expectations for the course is that you share ideas and opinions freely and that we identify a review paper, book review or some other form of class authored publication. Previous classes have published papers in BioScience (Choate et al. below), Trends in Ecology and Evolution (Prather et al. below) and book reviews for various journals.

Because of my travel schedule, our class meeting times will need to be flexible and mutually agreed upon. I will make as many of our schedule Tuesday meetings as possible, but there will be times when I cannot and we will need to meet twice during the weeks I am here.

Outline of Discussion Topics:

Discussion 1: A brief history of the philosophy of science.

Discussion 2: The scientific method in natural sciences: the realization that environmental science is not physics; Is statistics the answer?

Discussion 3: Is there a philosophy of Engineering?

Discussion 4: Is there a philosophy of Computer Sciences?

Discussions 5 - 8: The nature of theory.

Discussion 9 - 12: Integration of ideas and data.

Discussion 13: The Goals, challenges and importance of interdisciplinary knowledge.

References:

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Ford, E.D. 2000. Scientific method for ecological research. Cambridge University Press. Cambridge, United Kingdom.

Levin, J. R. 1998. What if there were no more bickering about statistical signifcance tests? *Research in the Schools* 5:43-53.

Osenberg, C. W., R. J. Schmitt, S. J. Holbrook, K. E. Abu-Saba and A. R. Flegal. 1994. Detection of environmental impacts: natural variability, effect size, and power analysis. *Ecological Applications* 4(1):16-30.

Prather, C.M., D.M. Choate and M.J. Michel. 2009. Putting the "Ph" back into the "Ph.D.": framing graduate research in a theoretical context. Frontiers in Ecology and the Environment 7:389-390.

Stewart-Oaten, A., Bence,J.R., Osenberg,C.W. 1992. Assessing effects of unreplicated perturbations - no simple solutions. *Ecology*: 73(4):1396-1404.

Van de Poel, I. 2009. Philosophy and Engineering: Setting the Stage. Volume 2: Philosophy of Engineering and Technology, P. 1-11.