ENATIONAL

RESEARCH ASSOCIATESHIP PROGRAMS

The Postdoc

Spring-Summer 2012

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IN BOTH WAR AND PEACE-

TIME SCENARIOS, fire in shipboard environment is serious and frequently results in excessive damage and high repair costs because the fire is not detected or controlled adequately. To help further improve future shipboard firefighting capability **senior scientists and NRC Postdoctoral Research Associates at the Naval Research Laboratory** (NRL) have formed an interdisciplinary team to develop a humanoid robot that could fight fires on the next generation of combatants. A humanoidtype robot was chosen because it was deemed best suited to operate within the confines of

NRL Firefighting Robot



Watch this! http://www.nrl.navy.mil/media/videos/nrl-damage-control-firefighting-operations

an environment that was designed for human mobility and offered opportunity for other potential warfighting applications within the Navy and Marine Corps.

The firefighting robot, called the **Shipboard Autonomous Firefighting Robot** (SAFFiR), is being designed to move autonomously throughout the ship, interact with people, and fight fires, handling many of the dangerous firefighting tasks that are normally performed by humans. The humanoid robot should be able to manuver well in the narrow passages and ladderways that are unique to a ship and challenging for most older, simpler robots to navigate. *continued on pg. 3*

"The Postdoc" highlights research and activities of NRC Associates and Advisers who participate in the agency/ laboratory programs with the NRC. Our newsletters are available in print and on our website: http://sites.nationalacademies.org/PGA/RAP/PGA_047804. Send all inquiries and submissions to Suzanne White (swhite@nas.edu)

NATIONAL RESEARCH COUNCIL OF THE NATIONAL ACADEMIES

NRC RAP Representation at 2012 Meetings

NAME OF MEETING	DATES	LOCATION	
Nat'l. Conf. on Race and Ethnicity in American Higher Education	05/29-06/02/2012	New York	NY
American Society for Microbiology	06/16-19/2012	San Francisco	CA
McNair Scholars Conference-University of Buffalo	07/21/2012	Niagara Falls	NY
STEM Annual Postdoc Conference and Career Fair (REDI)	07/12/2012	Bethesda	MD
American Chemical Society - Fall Meeting	09/10-12/2012	Philadelphia	PA
National Organization of Black Chemists and Chemical Engineers	09/25-28/2012	Washington	DC
Florida Education Fund-McKnight Fellows Conference	10/01/2012	Tampa	FL
Mexican American Engineering and Science Society	10/12-13/2012	Las Vegas	NV
Soc. for Advancement of Chicanos and Native Americans in Science	10/11-14/2012	Seattle	WA
Hispanic Association of Colleges and Universities	10/20-22/2012	Washington	DC
American Indian Science and Engineering Society	11/01-03/2012	Anchorage	AK
Annual Biomedical Research Conference for Minority Students	11/07-10/2012	San Jose	CA
American Society of Tropical Medicine and Hygiene	11/11-15/2012	Atlanta	GA
American Geophysical Union	12/03-07/2012	San Francisco	CA

Biologists develop new method to track young 'lost years' sea turtles



Dr. Kate Mansfield (former NRC Associate) & turtle prior to turtle's release in the Gulf Stream, 2009-Jim Abernethy

By combining everyday beauty products with scientific technology, **Kate Mansfield**, **Ph.D.** (**NRC Associate from 2009-2011**) a sea turtle biologist and visiting assistant research professor with **National Oceanic and Atmospheric Administration (NOAA) Southeast Fisheries Science Center and Florida International University**, along with Jeanette Wyneken, Ph.D., associate professor of biological sciences in the Charles E. Schmidt College of Science at Florida Atlantic University, developed a safe and reliable method of attaching small satellite tags to very small sea turtles. Otherwise known as the "lost years," very little is known about the behavior, movement patterns and habitat use of sea turtles from the time they leave the beaches as hatchlings until they show up again years later in coastal waters as juveniles or adults. The challenge faced by Drs. Mansfield and Wyneken was to develop a minimally-invasive way to attach a satellite-tracking device to small (<20 cm in length), fast-growing turtles. The tracking device needed to be small and light enough so as not to impair turtles' movements with an attachment that was robust but flexible enough to survive the turtles' rapid growth within a marine environment. Until recently, available battery-powered tag technologies were too large and heavy for these small animals.

The team began by testing marine epoxies and other adhesives typically used to track older, larger sea turtles for long periods in the open ocean (1-2 years). None of these methods worked on the small, fast-growing loggerhead turtles; the turtles shed the tag attachments within one to two weeks. The solution came from Dr. Wyneken's manicurist. Loggerhead sea turtle shells are made of the same substance as human fingernails: keratin. At the manicurist's recommendation, the researchers applied an acrylic base coat — the same product used in nail salons — to the turtles' shells, extending tag attachment durations up to 4-8 times longer than without the acrylic. Using small, solar-powered satellite tags (originally used to track birds) and a combination of manicure acrylic, hair extension glue, old wetsuits, and aquarium silicone, laboratory tests revealed that the devices remain in place for at least 60-90 days without altering the shell underneath.

After extensive laboratory testing, the researchers fieldtested the attachment method and tags' performance on laboratoryreared loggerheads released from southeast Florida. The tags performed very well in the field and were successful in providing the first long-term assessments of migration routes and habitat use by young loggerheads leaving Florida's east coast.

21st Century Damage Control continued from front cover

The robot is designed with enhanced multimodal sensor technology for advanced navigation and a sensor suite that includes a camera, gas sensor, and stereo IR camera to enable it to see through smoke. Its upper body will be capable of manipulating fire suppressors and throwing propelled extinguishing agent technology (PEAT) grenades. It is battery powered that holds enough energy for 30 minutes of firefighting. Like a sure-footed sailor, the robot will also be capable of walking in all directions, balancing in sea conditions, and traversing obstacles.



Virginia Tech m University of Pennsylvania, and NRL are working on the firefighting robot project. NRL's firefighting robot will be a follow-on version to the existing Virginia Tech: CHARLI-L1 robot.

Another key element of the SAF-FiR development is to allow damage control personnel and the robot to work cohesively as a team. Algorithms are being developed to allow autonomous mobility and decision making by the robot as a team member. To enable natural interaction with a human team leader, the robot will have multimodal interfaces that will enable the robot to track the focus of attention of the human team leader, as well as to allow the robot to understand and respond to gestures, such as pointing and hand signals. Where appropriate, natural language may also be incorporated, as well as other modes of communication and supervision.

NRC Research Associateship Programs Newsletter

Researchers from Virginia Tech and University of Pennsylvania are also working with NRL on the project. They plan to test the firefighting robot in a realistic firefighting environment onboard the ex-USS Shadwell in late September 2013. The Navy Technology Center for Safety & Survivability, located at NRL in Washington, D.C., carries out research aimed to solve current and future Navy problems regarding combustion, fire extinguishment, fire modeling and scaling, damage control, and atmosphere hazards. The Center has unique fire research facilities that include pressurable chambers up to a 10,000 cubic foot capacity at the Centers test site at NRL's Chesapeake Bay Detachment in Maryland.

The Center also has custody of the world's unique fire test ship, ex-USS Shadwell (LSD-15) located in Mobile, Alabama, where full-scale fire and damage control tests are conducted using the reality conformations of active duty sailors. Using the ex-USS Shadwell, NRL scientists are able to enhance their technology base for introducing advanced damage control concepts to the fleet. The ship provides a unique opportunity to realistically experience a true damage control environment, to create a partnership between the technical and fleet communities, and to take advantage of new insights gleaned during full-scale experimentation.

The Navy Center for Applied Research in Artificial Intelligence (NCARAI) has been involved in both basic and applied research in artificial intelligence, human factors, and human-centered computing since its inception in 1981. NCARAI, part of the Information Technology Division within NRL,

is engaged in research and development efforts designed to address the application of artificial intelligence technology and techniques to critical Navy and national problems. The NCARAI is developing the algorithms that allow the



Dept. of Defense (DoD)

NRL NRC Associates: Eric Martinson Laura Hiatt Mcgill Lilia Moshkina Thomas Apker NRC NRL Adviser: John Greg Trafton

firefighting robot to work naturally with human firefighters, as well as high-level reasoning capabilities.

The Laboratory for Autonomous Systems Research will provide specialized facilities to support highly innovative, multidisciplinary research in autonomous systems, including intelligent autonomy, sensor systems, power and energy systems, human-system interaction, networking and communications, and platforms.

The Laboratory will capitalize on the broad multidisciplinary

NY's Bronx River study explores use of nutrient bioextraction

Mankind has used lakes, rivers, estuaries, and coastal seas as dumping grounds for many pollutants, including nutrients that over-fertilize algae and plants leading to a condition known as eutrophication. There are different strategies to mitigate eutrophication, e.g. waste-water treatment plants, but there is a great interest in finding a green solution to recycle the excess nutrients already in coastal waters. Bivalve mollusks -oysters, clams, scallops, and mussels- capture microscopic particles, mainly phytoplankton, as a food source, thereby mitigating eutrophication and improving the water quality

The loss of native bivalve filtration in coastal and estuarine ecosystems through over-harvest and habitat destruction can result in the same ecological effects as eutrophication. The use of shellfish (bivalves among them) aquaculture to capture and remove nutrients in the coastal environment is thought to be as economically favorable as other nutrient reduction measures, such as agricultural best management practices or urban storm water retrofitting. The environmental management strategy by which nutrients are removed from an aquatic ecosystem through the harvest of enhanced biological production, including the aquaculture of suspension feeding shellfish or algae, is being called nutrient bioextraction. The specie to use in each area should be chosen carefully according to the characteristics of the water and endemic species displaced or depleted.

Within this context, my postdoctoral research has been to study the biology of the Atlantic ribbed mussel (Geukensia demissa) as potential specie for nutrient bioextraction purposes in Long Island Sound. The Atlantic ribbed mussel is found in intertidal habitats, mainly salt marshes, along the North American Atlantic Coast, Ribbed mussels are able to feed efficiently on particles suspended in the water and exploit many available food resources. This species also has unusual tolerance to dehydration, variation of salinity, and thermal stress, and it has much higher tolerance to sulfide than other bivalves. These adaptations enable this mussel to be the dominant benthic suspension feeder in salt marshes, playing a key role in the flow of nutrients in the ecosystems they inhabit.

The main goal of my research was

to study the feeding behavior of the ribbed mussel to determine, among other characteristics, how much they can filter and the efficiency with which they retain particles from the water. Moreover, my laboratory's group wanted to understand the regulatory mechanisms of the feeding behavior; in other words, observe the feeding plasticity of this mussel. For this purpose, in situ filterfeeding experiments were conducted in two very different environments: Milford Harbor (CT) and Hunts Point (Bronx, NY). Both study sites support naturally-occurring ribbed mussel populations, but are very different in terms of physics, chemistry and biology. The Bronx site is in a highly-urban, densely-populated, and industrial section of New York City.



Dr. Eva Galimany, NRC Associate, NOAA, "showing her mussels"

Hunts Point is located at the confluence of two rivers and is in close proximity to one of New York City's largest wastewater treatment plants (the Hunts Point Wastewater Treatment Plant, which releases 378-757 million liters of treated effluent per day). In contrast, Milford Harbor is located in suburban, coastal Connecticut, with lower resident population density, less industry, and much less riverine influence. My findings showed that ribbed mussels adapted feeding physiology to the different characteristics of the water characteristics of the two study locations. Despite the high particulate loads found at both Milford Harbor and Hunts Point, the water seston quality was very different between the two sites. Milford Harbor consistently had twice

the amount of organic matter as Hunts Point. Moreover, increased total particulates in Milford Harbor was attributable to phytoplankton blooms; whereas, increased total particulate matter in Hunts Point was associated with inorganic matter – mud from the bottom stirred up by tidal currents. Mussels adapted to these very different particle characteristics with different feeding strategies to reach, surprisingly achieving the same absorption efficiency of organic matter. Ribbed mussels in Milford Harbor decreased clearance rate with increased total particulate matter; whereas, the mussels in Hunts Point increased the time to process the food in the digestive system

> with increased particulates. These findings demonstrate the physiological plasticity of ribbed mussels and the wide range of inorganic content they can process.

To further study filtration plasticity, we moved ribbed mussels from Milford Harbor to Hunts Point and did the same feeding experiments with both populations at the same time. The mussels from Milford had a much lower absorption efficiency, which means that from the same food, they absorbed much less than ribbed mussels living near Hunts Point. Just 6 days after transplanting Milford mussels to Hunts Point, both populations reached the same efficiency proving again the highly adaptable feeding plasticity of ribbed mussels.

In addition to these relevant findings, we also ex-

plored other aspects of the biology of the ribbed mussel. Specifically, I conducted a histo-pathological study with monthly samples during an entire year from both sites, Milford Harbor and Hunts Point. This study revealed that both populations are synchronized with respect to reproductive biology. Moreover, both populations had very low incidences of disease and pathologies, indicating a healthy status of the individual mussels at both sites. The cultivation of ribbed mussels for bioremediation of eutrophication of coastal waters can employ typical suspension culture methods used world-wide to grow other mussels for human food.

continued on page 15



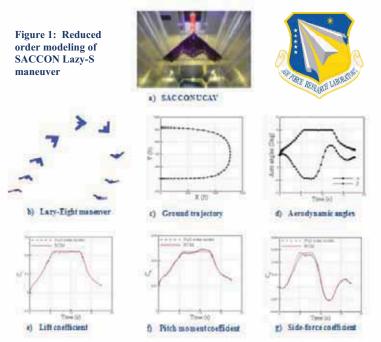
Reduced-Order Aerodynamic Loads Modeling of Maneuvering Aircraft

Dr. Mehdi Ghoreyshi, NRC Associate, and the Modeling and Simulation Research Center in the U.S. Air Force

Academy. Colorado, focus research on the prediction of aerodynamic loads. This remains a challenging engineering issue for military aircraft designers. Unsteadiness in the flow can lead to uncommanded motion and uncontrollable departure in flight testing. Despite their greatest efforts using the best available predictive capabilities, nearly every major fighter program since 1960 has had costly nonlinear aerodynamic or fluid-structure interaction issues that were not discovered until flight testing. Currently, the use of computational fluid dynamics (CFD) solutions is considered the state of the art in modeling unsteady nonlinear flow physics and offers an early and improved understanding and prediction of aircraft aerodynamic characteristics. Specifically, significant progress has been made by the US Air Force Academy (USAFA) and others in demonstrating the ability of Unsteady Reynolds Averaged Navier-Stokes (URANS) and Delayed Detached Eddy Simulation (DDES) approaches to accurately predict the forces and moments on aircraft maneuvering at the edge of the flight envelope. With the advanced computing techniques, one straightforward way to calculate unsteady aerodynamics forces and moments of a maneuvering aircraft is to develop a full-order mathematical model based on direct solution of discretized Navier-Stokes equations coupled with the dynamic equations governing the aircraft motion. However, a fullorder model for Stability & Control (S&C) analysis is computationally very expensive approach since such a model needs a large number of coupled computations for different values of motion frequency and amplitude. An alternative approach to solving the full-order model is to develop a Reduced Order Model (ROM) that seeks to approximate CFD results by extracting information from a limited number of fullorder simulations.

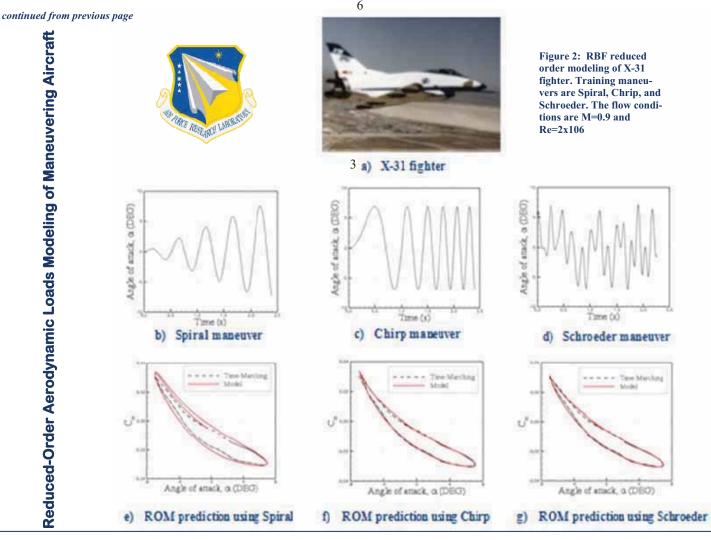
Dr. Ghoreyshi's research at USAFA, under the guidance of Prof. Russell Cummings, focuses on the development of ROMs using CFD to make timely progress in predicting and modeling unsteady loads of a maneuvering aircraft. The developed ROMs are based on indicial functions and Radial Basis Functions for different configurations. A linear ROM was created using indicial type CFD calculations (URANS) and used for predictions in order to check the validity of the ROMs for the SACCON UCAV undergoing a lazy-eight maneuver (Fig. 1). The comparisons between the created ROM with the fullorder model show good agreement in lift, pitch moment, and side force. The small discrepancies at high angles of attack are very likely due to the linear assumptions in the ROM, which will be addressed in the next phase of work. Note that the computational grid has around 13M cells and the cost of generating the full-order model is approximately 50,000 CPU hours using 512 processors. Once the ROM is created, the aerodynamic loads for maneuvers can be predicted on the order of a few seconds.

Also, the X-31 fighter undergoing pitching at transonic speeds for three different training maneuvers has been investigated. All maneuvers ran for 2.4 seconds and started from a steady-state solution. The aircraft responses to these maneuvers were generated using URANS equations. The cost of generating each response is around 138 wall-clock hours using 256 processors (2.3 GHz) for a half geometry mesh with 11.7 M cells. A ROM is created using Radial Basis Functions and was tested for prediction of a pitching motion at transonic speeds (Fig. 2). The results show that the predicted ROM values agree well with the full-order solution, with the ROM based on the Schroeder maneuver showing better accuracy than models based on the chirp and spiral maneuvers. Future work includes development of methods to select the best training maneuver for ROM construction in the frequency/amplitude/Mac/altitude space.





Dr. Mehdi Ghoreyshi, NRC Associate at AFRL



Turtles continued from page 2

"The methods we developed will revolutionize our ability to study the in-water movements and habitat use of very young, very small, oceanic stage sea turtles, a life stage known as the 'lost years' due to the lack of information on these young turtles," said Mansfield. "This work allows us to track a whole new size- and age-class of sea turtle. Population models rely heavily on data derived from older turtles or hatchlings that are more accessible to researchers within coastal and beach habitats. Tracking sea turtles during their first year at sea will allow us to fill in some of the gaps in our knowledge of early sea turtle life history. By identifying the movement patterns and behavior of oceanic stage turtles, we will ultimately be able to identify areas for targeted species management."

The study results will be published in a forthcoming issue of *Marine Ecology Progress Series*. This study was the main focus of **Dr. Mansfield's research as a NRC Research Associate based at the NOAA Southeast** **Fisheries Science Center in Miami, Florida.** This research was supported by several sources, including: the Ashwanden Family Fund, Disney Worldwide Conservation Fund, the Florida Sea Turtle Grants Program, Large Pelagics Research Center, National Academies Research Associateship Program, Nelligan Sea Turtle Fund, NOAA Fisheries, Save Our Seas Foundation and The Philanthropic Collaborative.



Dr. Mansfield is currently building on her NRC research by applying the methods she and Dr. Wyneken developed to other species of sea turtle and to wildcaught turtles in the northwestern Atlantic, Gulf of Mexico and southern Atlantic Ocean.



- ↑ Tagged turtles before release
 2009- Kate Mansfield
 ← Loggerhead turtle and satellite tag
- 2009-JimAbernethy ↓ A hard epoxy attachment method tested
- and rejected during laboratory trials 2009-Kate Mansfield



NRL researchers discover technique to improve solar cell technology

A multi-disciplinary team of scientists at NRL has discovered a way to tailor nanostructures that could result in lowcost, high efficiency solar cells. The research appears in the August 10, 2011 issue of the journal *Nano Letters*.

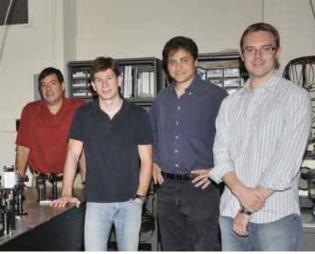
The technology behind optoelectronic devices currently in use has been limited by the fact that a single photon absorbed by a semiconductor results in the creation of a single electron-hole pair, or exciton. The NRL researchers have found that changing the shape of PbSe (lead selenide) nanostructures enhances a down conversion process known as multiple exciton generation. To accomplish this, the team uses elongated (cigarshaped) nanorods instead of spherically symmetric (ball-like) nanocrystals.

Unlike the current optoelectronic technology that relies on a single electron-hole pair per photon, in multiple exciton generation the excess energy of the "hot" exciton is used to excite a sec-

ond electron across the band gap resulting in the creation of two or more excitons per photon. The NRL team's discovery that this process is significantly more efficient in the elongated nanorod structures provides a new pathway to increasing the efficiency of solar cells over current stateof-the-art devices.

These elongated structures are the most efficient photon energy down

Drs. Edward Foos, Janice Boercker, and Anthony Smith (NRC affiliated) in the nanomaterial synthesis lab.

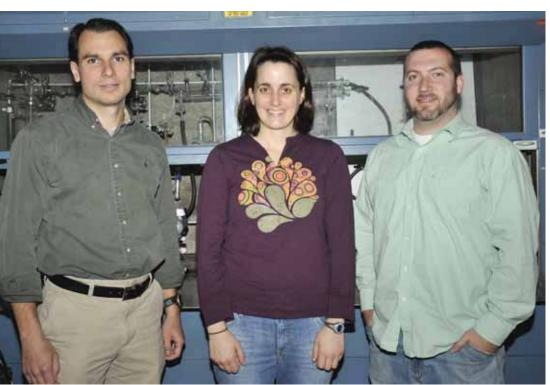


Drs. Joseph Melinger, Paul Cunningham, and Joseph Tischler (NRC-affiliated Associates or Advisers), and Matthew Lumb, next to a two-color femtosecond laser pump-probe apparatus is used to measure the efficiency of multiple exciton generation in PbSe semiconductor nanocrystals and nanorods.



converters known. As a result, this material system provides a way of harvesting solar energy extremely efficiently. In addition, the synthesis process is low cost, which would make these solar cells very inexpensive, and the materials are compatible with solution processing of devices on flexible substrates. Possible future applications emerging from this technology besides photovoltaic cells could include ultra-sensitive photo detectors, high-speed electronics, light emitting diodes, lasers, and biological labels.

The research team consists of Drs. Paul Cunningham, Janice Boercker, Joseph Tischler, and Joseph Melinger (NRC affiliated) and Matthew Lumb from NRL's Electronics Science and Technology Division; and Drs. Edward Foos and Anthony Smith (also NRL affiliated) from NRL's Chemistry Division.



Spring-Summer 2012

Spotlight on Podcasts

"Publishing Your Research 101"

http://pubs.acs.org/page/publish-research/ overview.html

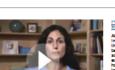


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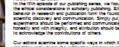


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Publishing Your Research 101 - bo. 2 Winting Your Cover Latter

About this episode

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Publishing Your Research 101 - Eq. 1 How to Write a Paper to Communicate Your Rese

South this episode he first episode in our series is an interview with Professor George M. Histolates from Harvard University who has guidated nearly 500 pages dh ACS Publications, and over 1100 articles ownal, and has served on the addrasy boards of rims gen-where jurnars.

Related Videox Improving your writing skills (2.56)

Writing to people will notice (4.05) White here you done when your writing is neglicien? (2.56) White any your frontie archites? (1.55) The impact of technology on scientific prices (3.51) Videas and scientific communication (3.55) How do you shotses your areas for research? (2.20) Why do your do the video? (2.11) **Full Audio**

Full interview, succo only (43:25)



Meet these Global Winners of YouTube Science Lab!

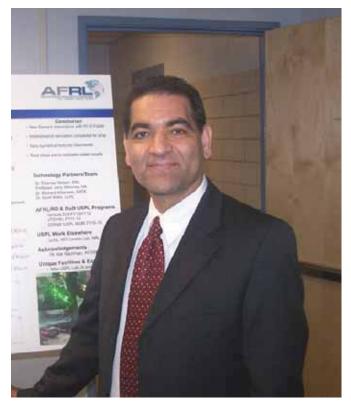
http://www.youtube.com/results?







Large-Scale Time-Intensive Computations



Dr. Mohammad R. Zunoubi, NRC Senior Research Fellow

continued from upper right



This development was significant as Professor Zunoubi's CUDA-MPI tool was able to interface simultaneously with multiple GPU's or linked stand alone systems containing GPU's, but even more significant is its ability to direct 32 and 64 bit personal computers/workstations simultaneously. The end result was the delivery of an efficient process that can achieve the realworld scenario of exposure to microwaves yielding the 1-mm resolution required in the Visible Human Project (VHP) anatomical man model with over 44 tissue properties and consisting of over 450 millions FDTD voxels. Prior to this, researchers at the AFRL/RHDR were using a 96-core processor CPU cluster to perform a frequency sweep calculation of the Specific Absorption Rate (SAR) of the 1-mm model in approximately 3 and a half days of computation time. The new tool developed by Professor Zunoubi performs the same calculations in a total of 194 minutes while providing an inhouse computational capability of unparalleled performance. To our knowledge, this is the very first time that such calculations have been accomplished without any form of traditional computational clusters.

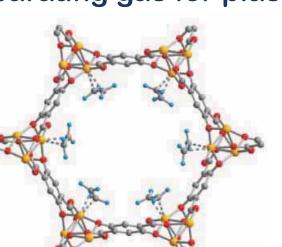
The work cited above was finalized while Professor Mohammad R. Zunoubi was a NRC Senior Fellow with NRC Adviser, Dr. William P. Roach from July 2011 through July 2012 at the Air Force Research Laboratory, Directed Energy Directorate, Laser Division, Advanced Electrical Laser Branch, Kirtland AFB, NM and supports directly the Ultrashort Pulsed Laser Programs computational efforts. The Air Force Research Laboratory, 711th Human Performance Wing, Human Effectiveness Directorate, Directed Energy Bioeffects Division, Radio Frequency Radiation Branch (AFRL/RHDR) is known as a premier research facility for studying the effects of high-power (HP) microwaves in human tissues. It was there that the first computational man model was created using the National Institute of Health Visible Human Project's anatomical data. Due to the extreme computational complexity, modeling the bioeffects within such models have traditionally required the use of a supercomputing facility which has a well documented history of high cost and long return times associated with their size and maintenance. In 2009, Dr. William P. Roach initiated the idea of using Graphic Processing Units (GPUs) as an alternative to the conventional CPU supercomputers to aid AFRL/RHDR's long delay times to receive critically needed data.

Through the Air Force Office of Scientific Research National Research Council (NRC) Summer Faculty Fellowship Program, Dr. Mohammad R. Zunoubi of SUNY, New Paltz, proposed implementing the Finite-Difference Time-Domain methodology for the dispersive media on a single GPU card. Although the initial effort showed significant promise for real-time analysis of human exposure to high power microwaves, it was soon realized that studying the bioeffects on a complete human model needed far more computational resources than a single GPU. Professor Zunoubi continued his effort on extending his implementations on multiple GPUs by using a combination of Compute Unified Device Architecture (CUDA), OpenMP (Massage Passing), and Message Passing Interface (MPI) Application Programming Interfaces (APIs).

The RDLAS Ultrashort Pulse Laser team's computational arm lead by Dr. Mohammad Zunoubi, Senior Fellow in the AFRL/NRC Summer Faculty Fellowship Program, SUNY along with Mr. Noah Wolfe, Senior Computer Engineering major at UNM, and Dr. William P. Roach, NRC Adviser, delivered a stateof-the-art computational tool to the 711th HPW/RHDR and RHDO, Fort Sam Houston, TX on Tuesday Feb. 21, 2012. This represents the culmination of a collaborative effort between the two laboratories, AFRL/RD and the 711th HPW/RHD that began in 2009. This tool is based on the Finite-Difference Time-Domain implementation of the Maxwell's equations and is massively parallelized through an RDLAS developed Message Passing Interface and Compute Unified Device Architecture technology. It is capable of studying real-world scenarios, in real time, of RF and HPM human exposure with 1-mm resolution using the National Institute of Health Visible Human Project anatomical man model with over 44 tissue properties. Prior to this delivery, researchers at the Fort Sam Houston were using a 96-processor CPU cluster to perform a frequency sweep calculation of the Specific Absorption Rate of the 1-mm man model in approximately 3 ¹/₂ days of intensive computational time. Our new tool performs the same calculations in a total of 194 minutes while providing an in-house compute capability. To our knowledge, this is the very first time that such calculations are possible in such short times without the need for any high performance com-

ttp://www7.national-academies.org/rap	NRC Research Associateship Programs Newsletter 10	Spring- Summer 2012
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New material cuts energy costs of separating gas for plastics and fuels



Cross-section of the iron-based MOF bound to six ethylene molecules, as determined by neutron diffraction. The MOF consists of a carbon (gray) and oxygen (red-orange) framework with iron atoms (yellow-orange) at strategic sites to bind the ethylene carbon atoms. The attraction between the iron and unsaturated hydrocarbons like ethylene (olefins) allows the MOF to adsorb these hydrocarbons, separating them from saturated hydrocarbons (paraffins) even at high temperatures. Credit: NIST and Jeffrey Long lab, UC Berkeley

A new type of hybrid material developed at the University of California, Berkeley, could help oil and chemical companies save energy and money – and lower their environmental impacts – by eliminating an energy-intensive gasseparation process.

Today, to separate hydrocarbon gas mixtures into the pure chemicals needed to make plastics, refineries "crack" crude oil at high temperatures – 500 to 600 degrees Celsius – to break complex hydrocarbons into lighter, short-chain mole-cules. They then chill the gaseous mixture to 100 degrees below zero Celsius to liquefy and divide the gases into those destined for plastics and those used as fuel for home heating and cooking.

"Cryogenic distillation at low temperatures and high pressures is among the most energy intensive separations carried out at large scale in the chemical industry, and an environmental problem because of its contributions to global climate change," said Jeffrey Long, a professor of chemistry at the UC Berkeley and a faculty researcher at Lawrence Berkeley National Laboratory.

Long and his UC Berkeley colleagues now have created an iron-based material – a metal organic framework, or MOF – that can be used at high temperatures to efficiently separate these gases while eliminating the chilling.

"You need a very pure feedstock of propylene and ethylene for making some of the most important polymers, such as polypropylene, for consumer products, but refineries dump a lot of energy into bringing the high temperature gases down to cryogenic temperatures," Long said. "If you can do the separation at higher temperatures, you can save that energy. This material is really good at doing these particular separations." "The research conducted by the Long group exemplifies the potential of MOF-based materials relative to olefin/paraffin separations," said chemist Peter Nickias, a Dow Fellow at Dow Chemical Company in Michigan who was not involved in the research. "More specifically, the ability of the reported iron-based MOF to separate a variety of unsaturated hydrocarbons from saturated species not only shows the versatility of the iron-MOF system, but also clearly reveals the potential of MOFs as alternative adsorbents."

In the chemical industry, ethylene and propylene are called olefins, while methane, ethane and propane are called paraffins.

Long and his colleagues at UC Berkeley, the National Institute of Standards and Technology (NIST) in Gaithersburg, Md., and the University of Amsterdam in the Netherlands report their findings in the March 30 issue of *Science*.

MOFs for natural gas purification

The iron-MOF is also good at purifying natural gas, which is a mixture of methane and various types of hydrocarbon impurities that have to be removed before the gas can be used by consumers. "These impurities can then be sold for other uses", Long said. "MOF compounds have a very high surface area, which provides lots of area a gas mixture can interact with, and that surface contains iron atoms that can bind the unsaturated hydrocarbons. Acetylene,

ethylene and propylene will stick to those iron sites much more strongly than will ethane, propane or methane. That is the basis for the separation."



Drs. Craig Brown and Wendy Queen, NRC/NIST affiliated Researchers

Nickias noted that increased supplies of natural gas from shale have provided more opportunity to extract and use ethylene and propylene from natural gas, and a variety of materials and approaches are being examined to cut energy use during the refining and purification of olefins.

"Significant energy savings could be achieved if a nondistillation separation could be implemented, or more realistically, the load on a cryogenic distillation unit can be reduced via upstream modifications to the process," Nickias said. \rightarrow

NRC Research Associateship Programs Newsletter

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Petroleum refined for the chemical industry is typically a mix of hydrocarbons, primarily twocarbon molecules – ethane, ethylene and acetylene – and three-carbon chains – propane and propylene. Cryogenic distillation separates these compounds – all of them gases at

room temperature – by liquefying them at low temperatures and high pressure, which causes them to separate by density. Ethylene and propylene go into plastic polymers, while ethane and propane are typically used for fuel.

The researchers found that when pumping a gas mixture through the iron-based MOF (Fe-MOF-74), the propylene and ethylene bind to the iron embedded in the matrix, letting pure propane and ethane through. In their trials, the ethane coming out was 99.0 to 99.5 percent pure. The propane output was close to 100 percent pure, since no propylene could be detected.

After the ethane and propane emerge, the MOF can be heated or depressurized to release ethylene and propylene pure enough for making polymers. of a carbon (gray) and oxygen (red-orange) framework with iron atoms (yelloworange) at strategic sites to bind the ethylene carbon atoms. The attraction between the iron and unsaturated hydrocarbons like ethylene (olefins) allows the MOF to adsorb these hydrocarbons, separating them from saturated hydrocarbons (paraffins) even at high temperatures.

"Once you saturate the material - with ethylene, for example – you shut off the valve, stop the feed gas, warm up the absorber unit and the ethylene would come out in pure form as a gas," Long said.

MOFs are like packed soda straws

Through a microscope, Fe-MOF-74 looks like a collection of narrow tubes packed together like drinking straws in a box. Each tube is made of organic materials and six long strips of iron, which run lengthwise along the tube. Analysis by Long's colleagues at the NIST Center for Neutron Research showed that different light hydrocarbons have varied levels of attraction to the tubes' iron. By passing a mixed hydrocarbon gas through a series of filters made of the tubes, the hydrocarbon with the strongest affinity can be removed in the first filter layer, the next strongest in the second layer, and so forth.

"It works well at 45 degrees Celsius, which is closer to the temperature of hydrocarbons at some points in the distillation process," said co-author Wendy Queen, NRC postdoctoral Research Associate at NIST who worked for six months in Long's UC Berkeley lab. "The upshot is that if we can bring the MOF to market as a filtration device, the energy-intensive cooling step potentially can be eliminated. We are now trying out metals other than iron in the MOF in case we can find one that works even better."

Long and his laboratory colleagues are developing iron-based MOFs to capture carbon from smokestack emissions and sequester it to prevent its release into the atmosphere as a greenhouse gas. Similar MOFs, which can be made with different pore sizes and metals, turn out to be ideal for separating different types of hydrocarbons and for storing hydrogen and methane for use as fuel. Long's other colleagues are UC Berkeley graduate students Eric D. Bloch and Joseph M. Zadrozny; Rajamani Krishna of the Van't Hoff Institute for Molecular Sciences at the University of Amsterdam; and Craig M. Brown (NRC Adviser), of NIST and The Bragg Institute at the Australian Nuclear Science and Technology Organisation in Menai, New South Wales.

The research is part of the Center for Gas Separations Relevant to Clean Energy Technologies, an Energy Frontier Research Center funded by the Department of Energy that focuses primarily on creating novel materials for capturing and storing carbon dioxide.



Energy Frontier Research Center at UC Berkeley Berkeley Lab to Develop Novel Materials for Hydrogen Storage

http://newscenter.berkeley.edu/2012/03/29/new-material-cuts-energy-costs-ofseparating-gas-for-plastics-and-fuels/ http://www.nist.gov/ncnr/filter-032812.cfm

RAP Session:

"I am a native of South Carolina and did my graduate work at Clemson University. I heard about the NRC program from my PhD advisor, Shiou-Jyh Hwu. While at Clemson, I worked on the synthesis and characterization of low-dimensional magnetic materials. Upon graduation, I had a desire to learn more about materials characterization, with the goal of becoming a more well-rounded scientist. I thought that the NRC program could provide me with an opportunity to



learn about neutron scattering, a useful tool for the characterization of a wide array of materials and a field in which I had zero experience.

During my time at the NCNR I have had the opportunity to learn about neutron scattering from Craig, an expert in the field, as well as work with new types of materials that include various porous adsorbents used in gas storage and separation applications. Further, the NCNR made it possible for me to work for 6 months at the University of California, Berkeley in Jeff Long's lab, which is among the best and most well respected MOF (metal-organic framework) groups in the country.

The NRC program and the opportunities provided to me by my current mentor and the NCNR has positively impacted my career. As for my future plans, I just accepted a new position that I will begin in a few months at the Molecular Foundry at Lawrence Berkeley National Lab in Berkeley CA. I will be working to help develop a new program that is focused on the synthesis and characterization of porous materials".



Novel Filter Material Could Cut Natural Gas Refining Costs From NIST Tech Beat: March 29, 2012

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Debra Rolison: dual honors for advancements in chemistry

Receiving two awards in the science of chemistry, **Dr. Debra Rolison, NRL/NRC Adviser** is recognized by the Society of Electroanalytical Chemistry for outstanding contributions to analytical chemistry and by the Chemical Society of Washington for expanding the scientific frontier of nanostructured materials.



Instilling enthusiasm for science and research, Dr. Debra Rolison is the recipient of the 2011 Charles N. Reilley Award and the Chemical Society of Washington Hillebrand Prize for contributions to the science of chemistry.

"Dr. Rolison is a natural leader and a creative and productive scientist, instilling enthusiasm for science and research in others," said Dr. John N. Russell, Jr., head, NRL Surface Chemistry Branch. "A common theme underlying all of her research has been a willingness to explore complex, nanostructured systems, a physicochemical environ that is by no means well-defined."

Presented March 12, at the 2012 Pittcon conference, the Charles N. Reilley Award - given in memory of one of the most distinguished analytical chemists of the 20th century - is sponsored by the Society for Electroanalytical Chemistry (SEAC), dedicated to promoting advances in both basic and applied research in electroanalysis, providing a venue for the exchange of ideas among researchers from academia, industry and government and recognizing the achievements and contributions of scientists who work in the field of electroanalytical chemistry.

The Hillebrand Prize, awarded March 22, is presented by the Chemical Society of Washington (CSW) and is awarded annually for original contributions to the science of chemistry. The Hillebrand Prize, named for one of Washington's most distinguished chemists, Dr. William F. Hillebrand, originated in 1924 and is the most prestigious honor given each year by CSW recognizing significant accomplishments in chemistry.

Rolison received a bachelor's in chemistry from Florida Atlantic University in 1975 and a doctorate in chemistry from the University of North Carolina, Chapel Hill in 1980, the same year she began her career as a government scientist at the U.S. Naval Research Laboratory.

Her research focuses on multifunctional nanoarchitectures for ratecritical applications such as catalysis, energy storage and conversion and sensors. Rolison's most recent research accomplishments lie in engineering facile transport of electrons, ions and molecules within ultraporous, high surfacearea, multifunctional materials.

Among her professional distinctions, Rolison is a Fellow of the American Chemical Society-ACS (2011 class), the American Association for the Advancement of Science-AAAS (2001), the Association for Women in Science (2006), and the Materials Research Society-MRS (Inaugural Class). She is a recipient of the R.A. Glenn (2007) and the A.K. Doolittle (2009) Awards from the Fuel and the Polymer Materials Science and Engineering Divisions of the American Chemical Society, respectively. She received national ACS recognition as the 2011

recipient of the ACS Award for Chemistry of Materials and is one of the 14 researchers profiled by the editors of Science as a major innovator in energy science.

Rolison is also noted for her leadership within the national and international scientific community through numerous activities that include organization of national and international symposia for a range of professional societies (ACS, AAAS, Electrochemical Society [ECS], MRS, and the Federation of Analytical Chemistry and Spectroscopy Societies [FACSS]), service on advisory panels including a National Research Council (NRC) committee leading to a classified report on nanotechnology for the intelligence community, serving as editor of SEAC Communications from 1997-2002 and as a member of the SEAC Board of Directors (1996-2001).

She was a guest editor of the July 2011 issue of the MRS Bulletin, which focused on electrical energy storage to power the 21st century, and was co-editor of an MRS Transactions "*Aerogels and Aerogel-inspired Materials.*" She recently represented the ACS Inorganic Chemistry Division on the ACS council and has been a national voice for diversity in science and engineering.

"Rising Star" Megan Sassin

continued on next page



Dr. Megan Sassin, a NRC Research Associate chemist at the Naval Research Laboratory, has been honored by the American Chemical society with a Rising Star Award.

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Dr. Megan Sassin, a NRC Research Associate chemist at the Naval Research Laboratory, has been honored by the American Chemical Society (ACS) with a Rising Star Award.

ACS's Women Chemists Committee has established the award to recognize exceptional mid-career women chemists across all areas of chemistry on a national level. This new award, created in 2012, is intended to help promote the retention of women in science.

Dr. Sassin's research interests are presently centered on the design, fabrication, and characterization of multifunctional 3D electrode architectures for energystorage applications, such as electrochemical capacitors, aqueous rechargeable batteries, and all-solid-state 3D batteries.

Dr. Sassin received her bachelor's degree in chemistry from Southwestern University, Georgetown, Texas, in 2001 and subsequently earned her master's (2003) and doctorate (2007) degrees in chemistry from the University of California, Irvine under the direction of Professor Reginald M. Penner. Her graduate studies focused on using electrode position to fabricate nanowirebased thermocouples, which demonstrate sensor response times on the order of microseconds. While at UCI, she also founded the Calcium chapter of Iota Sigma Pi and served as the president from 2005 to 2007. Sassin ↑

Naval Research Laboratory scientist and NRC Adviser, Dr. Frances Ligler, has been elected to the American Institute for Medical and Biological Engineering's (AIMBE) College of Fellows. Dr. Ligler was nominated by her peers and was elected by the full membership into the official College of Fellows Class of 2012 "for engineering automated biosensors for fast, on-site detection of pathogens, toxins, pollutants, drugs of abuse, and explosives."

Ligler is the Navy's Senior Scientist for Biosensors and Biomaterials and a member and past chair of the Bioengineering Section of the <u>National Academy of Engineering</u>. She earned a B.S. degree from Furman University and both a D.Phil. and a D.Sc. from Oxford University.

Currently working in the fields of biosensors and microfluidics, Ligler has also performed research in biochemistry, immunology, and proteomics. She has over 350 full-length publications and patents, which have led to eleven commercial biosensor products and have been cited over 7500 times.

Ligler is the winner of the Navy Superior Civilian Service Medal, the National Drug Control Policy Technology Transfer Award, the Chemical Society Hillebrand Award, the Navy Merit Award, the Naval Research Laboratory Technology Transfer Award, three NRL Edison Awards for Patent of the Year, the Furman University Bell Tower and Distinguished Alumni of the 20th Century Awards, and the national Women in Science and Engineering (WISE) Outstanding Achievement in Science Award. In 2008, Dr. Sassin joined the <u>Advanced Electrochemical</u> <u>Materials Section</u> at NRL in Washington, D.C. as an NRC postdoctoral fellow, working with staff scientist Dr. Jeffrey W. Long to design, synthesize and characterize nanostructured electrode architectures that are used to enhance the performance of aqueous asymmetric electrochemical capacitors.

She joined the Advanced Electrochemical Materials section as a staff scientist in 2010, under the direction of Dr. Debra Rolison, and was subsequently awarded the Jerome and Isabella Karle Fellowship to investigate three-dimensional architectures for electrostatic capacitors. She is a co-recipient of the 2009 Arthur K. Doolittle Award from the Polymeric Materials: Science and Engineering Division of the ACS, and is the author of several high-profile papers, including two invited review articles on the topic of electrochemical capacitors.

Dr. Sassin and the other 2012 Rising Star Award winners were recognized during the recent national meeting of the American Chemical Society.



Fran Ligler elected to American Institute for Medical and Biological Engineer's College of Fellows

NRL's Dr. Frances Ligler is elected to AIMBE's College of Fellows.

Ligler serves as an Associate Editor of Analytical Chemistry and on editorial/advisory boards for Biosensors & Bioelectronics, Analytical Bioanalytical Chemistry, Sensors, Open Optics, and Applied Biochemistry and Biotechnology. Elected an SPIE Fellow in 2000, she also serves on the organizing committee for the World Biosensors Congress and the permanent steering committee for Europt(r) odes, the European Conference on Optical Sensors. In 2003, she was awarded the <u>Homeland Security Award</u> (Biological, Radiological, Nuclear Field) by the Christopher Columbus Foundation and the <u>Presidential Rank of Distinguished Senior Professional</u> by President Bush.

AIMBE's College of Fellows is comprised of the top two percent of medical and biological engineers in the country. Engineering and medical school chairs, research directors, innovators, and successful entrepreneurs, comprise the College of Fellows to pursue AIMBE's mission to provide leadership and advocacy in medical and biological engineering for the advancement of society.

Since 1991, the College of Fellows has led the way for technological growth and advancement in the fields of medical and biological engineering. Fellows have helped revolutionize medicine and related fields in order to enhance and extend the lives of people all over the world. They have also successfully advocated for public policies that have enabled researchers and business-makers to further the interests of engineers, scientists, and ultimately, patients.

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continued from pg 4 Dr. Eva Galimany at the Bronx River site. Constant submersion underwater is different than this species' natural, intertidal habitat in which they are exposed to a twice daily tidal regime of immersion and emersion. To assess possible effects of constant submersion upon the feeding behavior of the mussels, we quantified filter-feeding activities of ribbed mussels collected from either an intertidal location or a permanentlysubmerged population in the same embayment. Results show that mussels taken from the intertidal population had significantly-higher filtration than the submerged population initially, but after 3 days of submersion, this difference disappeared. These results indicate, once again, the plasticity and adaptability of this mussel species.

Toxic microalgal proliferations in aquatic ecosystems, referred to as Harmful Algal Blooms (HABs), appear to be increasing in geographic distribution and intensity, disrupting coastal and marine ecosystems and the organisms living there. Bivalves that are filter-feeders ingest noxious and toxic algae present in the water. Despite the ecological importance of ribbed mussels, and the documented impacts of HABs upon other filter-feeding shellfish, we found a lack of information regarding impacts of harmful algal species upon the health and filtration activities of G. demissa. The lack of studies on toxic algal interactions with ribbed mussels probably is because this bivalve is not harvested as a fishery product. We investigated the clearance rates and pathology of ribbed mussels exposed to cultures of two toxic algae, Aureococcus anophagefferens or Heterosigma akashiwo, and contrasted the results with mussels fed a non-toxic alga. We also conducted a separate, in vitro experiment in which we exposed extracted mussel hemocytes to the three different algae, respective culture media, and seawater, as a toxicity bioassay. Results show that mussels exposed to either of the toxic algae had decreased clearance rates during the entire exposure period; nevertheless, as opposed to other bivalves, ribbed mussels continued to filter the algae from the water. Ribbed mussels exposed to harmful algae had thinner digestive tubules, gonad reabsorption, and a decrease in gill ciliates compared to non-toxic controls.

We also observed an increase in mortality of hemocytes exposed in vitro to both toxic algae compared to seawater controls, demonstrating the cytotoxicity of the algae. Results suggest that ribbed mussel feeding behavior and physiology can be impacted in several ways by harmful algae, which could undermine their role in nutrient bioextraction.

RAP Session:

"All the findings during my postdoctoral experience demonstrate that ribbed mussels have a very flexible feeding physiology and unique abilities to adapt to local conditions making ribbed mussels a good candidate for nutrient bioextraction purposes in the North American Atlantic Coast. Nevertheless, during these two years of research I have learned many other things that have helped me grow as a scientist and as a person. Scientifically, I have learned many things such as to planning my work according to tides as opposed to the Mediterranean Sea, where I had previously developed most of my research.

I have also learned to work with a big group of people and that the combination of everyone's skills and will to help have made all my research possible, I'm very thankful to the NOAA Milford Laboratory colleagues. As a person, I have *learned that my plasticity can be compared to the one* found for ribbed mussels, adapting my life and family to a new environment, new language, and a very different way of life, which we have really enjoyed."



"This project in the Bronx River is one of the first to test the effectiveness of a relatively new technology," said Gary Wikfors, Milford's Biotechnology Branch chief and NEFSC project leader for the mussel study. "The idea has been successful in other countries, and if the pilot study goes well, shellfish aquaculture for nutrient removal could be applied in many other coastal environments."

"There is already considerable local interest in and 'buzz' about the project," Rose said. "We don't have any results yet since the project just got underway. The raft survived Hurricane Irene just days after it was installed in the river, and things have gone well so far, so we're off to a good start."

Long Island Sound Study=Nutrient Bioextraction Overview: http://longislandsoundstudy.net/issues-actions/water-quality/nutrientbioextraction-overview/ Rocking the Boat: http://www.rockingtheboat.org/

Milford Laboratory: http://mi.nefsc.noaa.gov

SPIE Optics Photonics conference (August 2012) invites Dr. Kenneth Marr. NRC Postdoctoral Research Associate at NRL: "Quantification and modeling of the thermal behavior of a laboratory DASH interferometer"

Temperature changes in a Doppler Asymmetric Spatially Heterodyned (DASH) interferometer cause variations which can be tracked and subsequently corrected during data analysis. Nonetheless, a quantitative understanding of the physics driving these effects is important for future instrument designs. In this study we constructed an interferometer with separate optical components which are allowed to expand independently with temperature. Thus, by measuring the thermally induced change to the interference pattern generated by this interferometer, we may characterize the thermal behavior of the system and validate the physics included in the simplified raytrace model.



Dr. Ken Marr, NRC Associate

May Review

2012 SCHEDULE

February Review

February 1 February 15 March 12-13 March 20

May 1

May 15

June 22

June 29

Application deadline Support doc deadline Panels/Review Board Results available to applicants

Application deadline

Support doc deadline

Results available to applicants

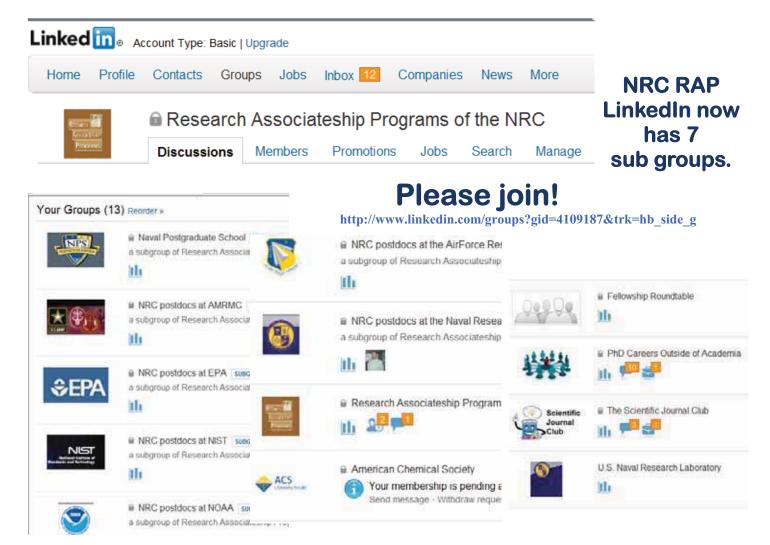
Review Board

August Review

Application deadline Support doc deadline Review Board Results available to applicants

November Review

Nov 1 Nov 15 January 7, 2013 January 14 Application deadline Support doc deadline Review Board Results available to applicants



Attention Advisers

We have substantially simplified the annual Research Update process for 2012. Instead of revising the Research Opportunities, we are asking you to update your contact information. If you haven't already, you will soon receive a secure link to the Contact Module. A username and password is no longer required.

Here's a brief summary of the process. After you receive your link, just click on View/Confirm to review your contact information. If everything is correct, choose "Confirm" and you are finished; no further action is required. If you need to make changes to your contact information, you may edit the appropriate section, save your changes, and then click "Confirm". You will have three months to complete this process.

While you are not required to review your Research Opportunity(s), you may update it now or at any time during the year. You would use the same secure link and go to the Opportunity Management Module.

Our goal is to keep the Web site up to date and this new procedure should enhance that process. We appreciate all the work you do to help us make this new procedure a success.