Department of Scientific Computing

Summer 2009

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On Assignment: Nymeyer Explores Lebanon while Teaching in Beirut

This past Spring, Assistant Professor Hugh Nymeyer was invited to teach at AUB, American University of Beirut. During April and May, he spent five weeks in Lebanon teaching biophysics, exploring Lebanon, surrounding cities and famous landmarks, and taking in the area culture and nightlife. The trip turned out to be quite an adventure, and he related his experiences both in and out of class.

Opportunity

"Tim Logan, the head of Molecular Biophysics (IMB) asked me if I wanted to go to AUB and teach a class. Two years ago Piotr Fajer went, and in past years Joe Schlenoff has gone and taught. IMB and Chemistry get a lot of grad students from AUB, so it's sort of publicity and recruiting for the university. In fact one of the students from my class is coming here in the Fall and will be a student in the Molecular Biophysics program."

The Course

"So there were eight students: six master's students, two Ph.D students, mostly from Lebanon. One of the girls was from Syria, which is fairly close. It's a two and a half, maybe a three hour drive to Damascus. Syria is much bigger and has a much bigger population. So one of the students in my class was Syrian. All the rest were Lebanese.

"It's a required course for them. It's a grad level biophysics class, so we talked about some structural things, like structures of proteins, chemical structures, amino acid structures, kinds of secondary structure. I talked about basic thermodynamics, unimolecular kinetics, biomolecular kinetics. Talked about molecular forces, hydrophobicity, electrostatic effects of membranes, some experimental methods. Class was one hour and fifteen minutes a day, five days a week."

Language

"So there's a written Arabic and there's a spoken Arabic, and spoken Arabic is really different depending on where you are. Here in the US, I think they mostly teach Egyptian pronunciation. So it sorta would be almost useless if you would go there, because they would not understand.

"Many people in Beirut speak English and French. A lot of people go to American schools or English schools and a lot of people go to French schools."

People

"The thing about the country is there's such a strange mix of people. You find a lot of people who are very western looking. You might find a woman with blonde hair, and she'll be right next to someone who's dressed with a head scarf but is sort of western dressed – like with slacks and a blouse. Then you find there are some people who wear black slacks and a top then they put a colored top over it and a

(Continued on page 7)

Max Gunzburger, DSC Chair

From the Chair

The Department of Scientific Computing has completed a very successful first year and all associated with the Department are expecting even more and better things in the coming year.

Our graduate degree programs continue to be attractive to students. Our incoming class numbers over a dozen students with, as has been the case in the past, very diverse disciplinary backgrounds but all with the common interest in learning how to develop improved methods for using computers to solve scientific and engineering problems.

Several of our graduate students spent the summer at national laboratories; we will feature their experiences in the next newsletter.

Perhaps the most important endeavor a department partakes in is the tenure and promotion process. I am very pleased that we went through this process without a hitch with Peter Beerli, who indeed was awarded tenure and promoted to the rank of Associate Professor. We were fortunate that our first case was very strong, which certainly made things easier for us. As the Chair, I look forward to piling on more duties on Peter, now that he is a tenure faculty member. (Just kidding, or not?)

The major task we will undertake in the next year is to prepare for the implementation of an undergraduate degree program in computational science. We hope to gain approval for the program this Fall, and then spend the Spring semester designing courses and recruiting students.

Chair, Department of Scientific Computing

Visiting Undergrads Research with DSC Faculty

Remember summer, those sweet endless days of recreation, exploration and discovery? For undergrads interested in science and computation, the meaning of summertime adventure is being redefined by Sachin Shanbhag, Anter El-Azab, and the new Research Experience for Undergraduates program in Scientific Computing. The program is sponsored by the National Science Foundation and invites undergraduates from across the nation to apply to spend the summer doing research in surface science, biology or nanoscience.

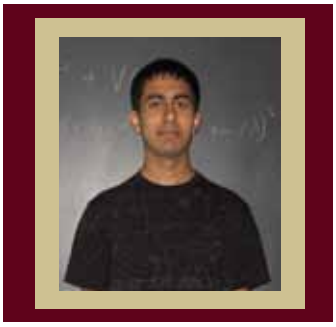
"The REU program in Computational Materials Science involves four different universities. A colleague at the University of Florida (UF) wrote an NSF grant to initiate and sponsor the program," said Shanbhag, an assistant professor in the Department of Scientific Computing who helped organize and launch the program. The grant came about as an outgrowth of the Florida Society for Materials Simulation, an alliance between Florida State, the University of Central Florida, UF and the University of South Florida. The organization's goal is to promote collaboration and education in materials science in universities throughout the state. After the grant award, a website announcing the goals, focus and parameters of the program was launched, and undergraduate students across the nation applied to the program.

"We have three students here. Michael Ericson from the University of Rhode Island is working with me to study polymers and how they deform under certain conditions. The other students at FSU are Ashley England and Ameet Gohil," said Shanbhag. Ashley is a senior from Illinois College who is working with Anter El-Azab; Ameet, also a senior, works with Wei Yang in Chemistry.

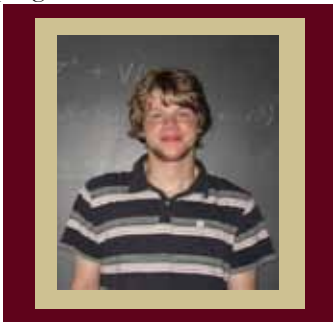
The program began in late May with orientation at each of the four individual campuses. Students and faculty then traveled to Gainesville for a meeting of all program participants. Materials science faculty at UF sponsored introductory lectures on computational simulations, modeling methods, ethics, career options and conducted a survey of the students regarding their expectations. After the lectures and a cookout, faculty and students returned to their respective campuses to begin the real work of the summer, including daily research, simulations, programming and data analyses, weekly presentations, laboratory tours and communications workshops.

REU will conclude the last week of July with the FSMS meeting at UF. The students will give presentations and poster sessions, and select faculty will facilitate materials science workshops. The program will continue until 2013.

Ashley England is a chemistry major from Illinois College, a small college (900 students) in Jacksonville, IL. Ashley is working with Anter El-Azab, extending research he has done with Srujan Rokkam. In her research, she is studying how metal oxides behave under certain conditions.



Ameet Gohil is a senior at the University of Iowa majoring in physics and electrical engineering. Ameet's project includes coding using the overlay method. He is trying to find an efficient way to figure out the geometry of a space using Baysian inference and Markov chains under the direction of Wei Yang.



Michael Ericson is a sophomore chemical engineering major at the University of Rhode Island. Michael is working with the architecture of low density polypropylene. His summer research is focused on the rheology of polymers, or how polymers respond to deformation. He works with Sachin Shanbhag.

Alan Lemmon, Assistant Professor

Phylogeography

Field Research

MIGRATION

Speciation

BIOLOGICAL SCIENCE

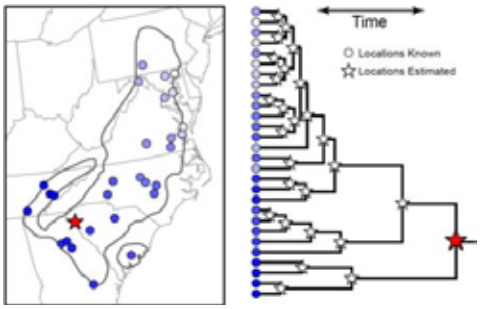
High Performance Computing

GENETICS

BIOLOGICAL SCIENCE

Geography and History Impact Species Formation

Since childhood, Alan Lemmon has been fascinated with the outdoors, animals, and natural habitats. With ingenuity, science and a little luck, he now parlays that fascination into a career that combines outdoor adventures with meaningful research. Lemmon studies phylogeography, or the way climate and geography have influenced species and their current distribution. Phylogeography uses DNA data to reconstruct geanological lineages, and the evolutionary history of species. The field is young, and has enjoyed changes in the last few years that make now a particularly exciting time for phylogeographic research. "Researchers in all fields of biology that use genetic data are on the verge of an exciting new frontier that is being thrust upon them by recent breakthroughs in genome sequencing technology. Whereas a large proportion of effort has traditionally been spent on data collection, the overwhelming majority of effort will soon be spent on data analysis. As a result, researchers and methods capable of integrating large quantities of complex data are already in short supply." The scope and depth of Lemmon's research has been enhanced from this breakthrough in data collection, allowing him to concentrate more intensely on speciation and how species are formed.

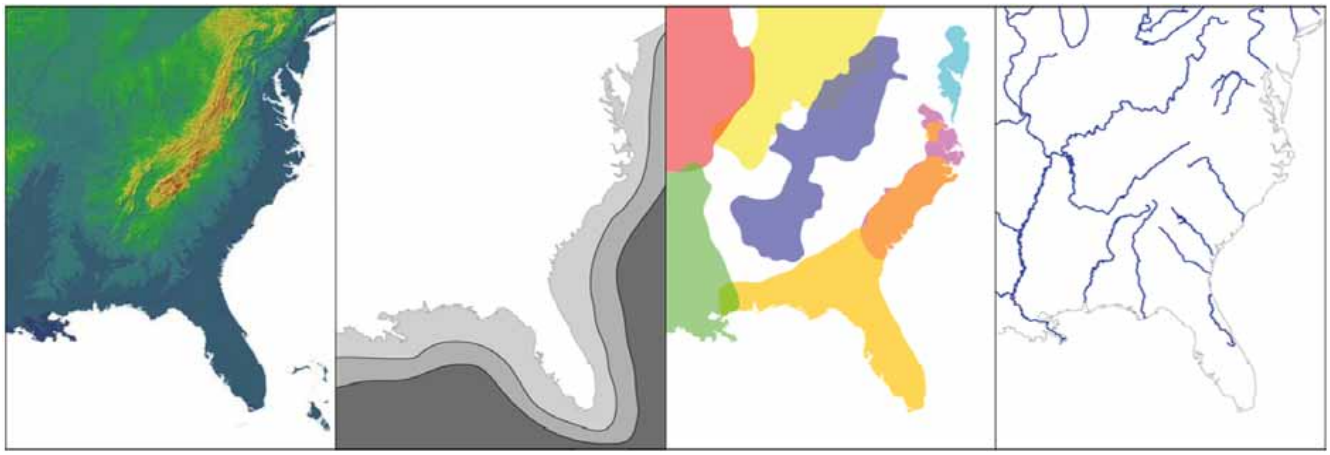


Estimating the phylogeographic history of *P. feriarum* in a maximum-likelihood framework. Data include the geographic coordinates of sampled individuals (left panel) and an estimated gene tree.

Speciation is thought to occur when biotic or abiotic factors cause geographic isolation of populations, which inhibits migration and allows for genetic divergence. When elements of the earth's physical structure - rivers, mountains, deserts or the like - isolate different species they interact and create new species. Quantifying the relative importance of different factors restricting gene flow is one of the most difficult aspects of studying speciation. "The study of genetic variation across geographic space is at the forefront of speciation research. Methods that can integrate the new types of genetic data with GIS data will have the potential to reveal important new insights into the process of speciation."

To study speciation and related subjects, biological scientists have used two complementary methodologies: a genealogical approach and a population genetic approach. The genealogical approach uses spatial distribution of sampled individuals to connect patterns of genetic variation to the processes that drive these patterns. In the population genetic approach, population sizes and migration rates are the primary focal point. The aim of this approach is to understand how and why demographic parameters have changed over time. Both of these approaches, however, have limitations that obstruct the integration of genetic and geographic data. Development of a new statistical framework that integrates characteristics of the two approaches would greatly increase the rigor and utility of the resulting research.

Lemmon's interest in developing and using software to teach and learn dates back to his days as an undergraduate, where he developed Evo-



Four potential barriers to gene flow will be incorporated into the analyses. Elevation data, (a), will be used to specify elevations greater than 450m as unsuitable. Estimates of coastlines, (b), from multiple time periods during the history of *P. feriarum* will be used to specify unsuitable geographic areas. Geographic ranges of species closely related to *P. feriarum* (species A-G), (c), will be used to identify regions of geographic space in which gene flow may be reduced due to species interactions (e.g., competition). Locations of major rivers will be used to define potential barriers to gene flow.

Tutor, partly as an outlet to channel his intense interest in evolution, and partly as a way to assist his classmates with understanding population genetics and speciation. Inspired by good professors and curiosity about how living things change over time, he continued his studies in graduate school and now devotes his research to studying how geographic barriers affect species. Knowledge of the processes that drive diversification of species not only helps us further our understanding of natural history, but also helps us make decisions on which geographic areas are most important to conserve.

Since becoming an assistant professor, Lemmon has been using these prior experiences to create PhyloMapper, software he and a collaborator are writing to support and refine their research and the research of others in their field. PhyloMapper includes functionality not currently found in other phylogeographic software packages. The software incorporates a Bayesian statistical framework, allows prior information (e.g. known geographic constraints on the species' range) to be utilized, enhances the power of hypothesis tests, makes quantification of uncertainty more intuitive, and allows the integration of geological (e.g. the specific location of rivers and mountains) and genetic data. Biologists can use it to test a diversity of explicit hypotheses about historical routes of migration, refugia, and geological factors contributing to speciation, as well as identify areas of high genetic diversity that should be targeted for conservation.

The field of phylogeography is certain to advance, as improved research capability coincides with increased interest, enhancements in the quantity and quality of data and the use of more sophisticated functionality in software. Lemmon is looking forward to being at the forefront of these developments in a profession that allows him to study a subject he has so long enjoyed.

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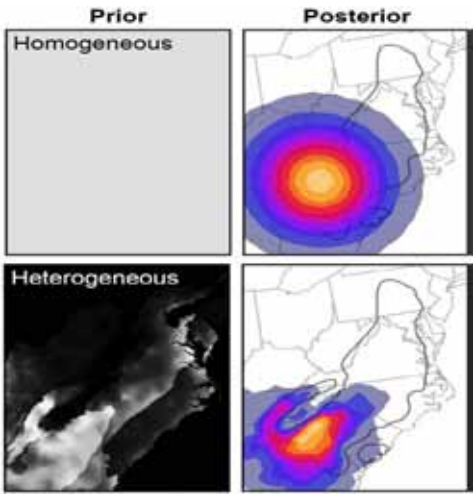

Accommodating environmental suitability improves estimates of phylogeographic history in a Bayesian framework. When a uniform prior is assumed for the location of the basal ancestor (top row), the posterior estimate is broad and includes unreasonable parts of parameter space (e.g. the ocean). When a heterogeneous prior is used (brightness corresponds to environmental suitability as estimated by an ecological niche model), the posterior estimate is much more precise. A statistical test using Bayes factors (BF) indicates that the heterogeneous prior is a better fit to the data.

With Summer come new Post Docs

New post-doc MEHMET ALI AKINLAR comes to Scientific Computing from the University of Texas at Arlington, where he completed his Doctor of Philosophy in Mathematics under the direction of

Guojun Liao. Mehmet's Bachelor and Master of Science degrees are also in Mathematics, and were obtained from the Anatolia University in Turkey (1999) and McMaster University in Canada (2002), respectively. Mehmet has been a teaching and research assistant for nine years. His research interests are in variational methods, control optimization, numerical computation and exact and numerical solutions of partial differential equations and their applications to industry. He will be working as a postdoctoral research assistant with Max Gunzburger. Mehmet is single, and enjoys intelligent discussions, traveling, and reading mathematics books.

QINGSHAN CHEN, one of Max Gunzburger's new post-docs, graduated with a BS in mathematics from Fudan University in Shanghai, China. He received his Masters and Ph.D. from Indiana University where he majored in Mathemematics and minored in Scientific Computing. His research centers on initial and boundary value problems for partial differential equations arising from physics and engineering, geophysical fluid dynamics, numerical methods for partial differential equations (finite difference, finite elements, spectral methods). Qinshan is published in the Journal of Computational Physics and Analysis and Applications and has taught undergraduate courses in trigonometry, calculus and finite mathematics. He and his wife, Yuefeng, are expecting their first baby.

XIAOMING HE arrived this Summer with a newly minted doctoral degree in Mathematics from Virginia Tech. Xiaoming holds a BS and a Masters Degree in Computational Mathematics from Sichuan University in Chengdu, China, and a Masters in Mathematics from Virginia Tech. Xiaoming's research focuses on finite element methods for partial differential equations and their applications, such as immersed finite elements for interface problems, finite element methods for the Stokes-Darcy system, splitting extrapolation, and Particle-in-Cell simulation for electrostatic levitation of lunar dust. He has co-authored many articles, and his research is published in the Journal of Computational Physics, Communications in Computational Physics, Numerical Methods for Partial Differential Equations, and IEEE Transactions on Plasma Science. In addition to publications, he has won several academic awards and presented at conferences. Xiaoming works with Max Gunzburger.

Originally from Russia, ALEXANDR LABOVSKY received his undergraduate degree in Applied Mathematics and Computer Science at Moscow State University. He completed his doctoral work at the University of Pittsburgh in Pennsylvania, and did a postdoc at the University of Missouri, Columbia in 2008-2009. Alex's general research interests include computational fluid dynamics, turbulence models for Navier-Stokes and coupled NS systems, numerical methods for partial differential equations and the dynamical systems approach to turbulence. Currently he is working on a project in Stochastic PDEs. Alex is married, and enjoys playing soccer and racquetball. He works with Max Gunzburger.

(Nymeyer, continued from page 1)

matching headscarf. Then there are some people who wear a long coat - which has to be beastly hot in the summer - a long coat and then the head scarf. And then there are some who wear a black dress scarf and just the face shows. There are some, not many, who wear the chodor with just the eyes showing. But it's strange because they're all right next to each other. And they're all ok with that."

Adventure

"There was this area I did go to but they told me I probably shouldn't have. There's an old Roman temple complex called Baalbek. It was their Phoenician Temple to the Sun. When the Romans came and took it, they made it the Temple to Jupiter, so from about 100 BC to 300 AD they kept building this place. The Temple to Jupiter is still completely standing except for the roof which was made of wood. It's really spectacular and it's massive. But that area of the country is a Hezbollah area, and I actually got lost.

"The students were going to go with me, and I figured they're all busy, and it was getting near the end, so I decided I'm just going to go. Well, I missed the turn at Chatura, and I went further, and I think to myself, 'Oh! I must have missed the turn.' Then I saw this blue sign that said Baalbek that way. So I thought, 'I'll just take that road.' As I'm driving along, the road is getting smaller and smaller and I'm hitting little potholes and I think, 'Hmmm, this isn't good.' Then I start going through these little towns, and every little town, you don't just go through the town, you have to take detours. These towns were definitely poorer than where I was, but not super rundown. They looked ok. But then I got to places that were more and more Hezbollah. And then I got to this town and they had Hezbollah flags flying everywhere, and I'm like, 'Oh Man! I'm turning around! I'm getting outta here!' And so I turned around and then I think, 'Crap! I'm not gonna make it to Baalbek!' But on the way back, I saw the big sign on a big road that had three lanes in each direction that said Baalbek and I said, 'Oh! That's the road!' And sure enough you just take that road and it's right there."

Night Life

"In front of the University is a street called Blitz Street. Blitz is just a whole place of food, food, coffee, ice cream, food! And that place, man! You go at midnight and they're triple parked. EVERYBODY's there. The first week I was there I was so out of it. I taught at 8 o'clock in the morning so I would get in and I would teach from 8 to 9:15 and then I would think, 'I gotta go home! I gotta go home and sleep!' So I would go home, and I would sleep until 2 in the afternoon. Then I would come in and work until 8 o'clock (pm) and then I would go out for dinner and then….. By the end I was a little bit better. But I don't know when they sleep! They all seem to be working in the morning at 8 o'clock."

Food

"For breakfast the big thing they eat is called manouche. It's thin bread that they put things on and then roll up like a sandwich. It's sort of like thin pita bread and usually nice and warm. The simplest thing they put on it - and they put this on everything - is called zatar. It's wild thyme and sumac. I actually brought a bunch back. It tastes sort of like thyme and oregano and they put that with olive oil on there. It's supposed to be good for your memory. So eat more zatar."

For more photos and an audio clip, go to www.sc.fsu.edu/

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The department's mission is to be the focal point of science and computation at Florida State University. Max Gunzburger is the Chair of the Department of Scientific Computing. He can be reached at 850.644.7024. Newsletters are issued three times each year. Subscriptions and single copies can be requested from Risette Posey, at 850.644.0196. This publication is available in an alternative format on request.

DSC Faculty Receive Stimulus Funds

When President Obama signed a $738 billion stimulus bill to assist the nation during the current recession, DSC faculty seized the opportunity to apply for the stimulus funding and have been rewarded for their efforts.

Tomek Plewa was awarded $380,000 from the Department of Energy to develop FLASH code and to contribute to the design, interpretation, and application of experiments conducted at the Center for Laser Experimental Astrophysics research. The grant funding will be used over a five year period to compare numerical results against experiments, to validate code, and provide feedback for better development. As the numerical tools mature, modeling of progressively advanced science problems will contribute to planning future experiments.

Jim Wilgenbusch and Paul Van der Mark received a three-year grant for personnel, equipment, travel and consultation services to facilitate the use and development of Bayesian methods to infer phylogenies. The group plans to create user-friendly software for practitioners to explore convergence of Markov chains generated by popular Bayesian phylogenic software packages. The same software will be made to output data in formats that are easily imported into other popular software packages so theoreticians unfamiliar with phylogeny software can more easily contribute to work in this area. The grant award is from the National Science Foundation and is $350,000.

Max Gunzburger is collaborating with colleagues from Colorado State and Penn State to transform how climate system models are used. The award recipients plan to (1) develop and evaluate methods for transitioning between parameterized and high-fidelity dynamic and tracer models as the grid transitions between coarse and fine regions, (2) develop goal-oriented optimization approaches that systematically and automatically determine where refinement is needed in order to obtain accurate simulations of dynamic and tracer transport in regional ocean modeling, (3) develop efficient, accurate and robust time-stepping schemes for variable spatial resolution discretizations used for regional ocean modeling of dynamics and tracer transport, and (4) develop frequency-dependent eddy viscosity finite element and discontinuous Galerkin methods and study their performance and effectiveness for simulation of dynamics and tracer transport in regional ocean modeling. The award from the Department of Energy is $226,000.