DEPARTMENT OF

Scientific
COMPUTING

FALL 2008

FACULTY PROFILES

Peter Beerli
Gordon Erlebacher
Anter El-Azab
Max Gunzburger
AlanLemmon
Anke Meyer-Baese
Michael Navon
Gavin Naylor
Hugh Nymeyer
Janet Peterson
Tomasz Plewa
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Xiaoqiang Wang
James Wilgenbusch
Ming Ye

New Department of Scientific Computing Approved

You've surely noticed the change in the newsletter banner that reflects the big change that occurred on August 8, 2008 -- the School of Computational Science is no more and now we are the Department of Scientific Computing! We are a full-fledged tenure granting department within the College of Arts & Sciences. It is the first such department at a research university in the US. The new department fulfills the real need, as delineated in several blue ribbon panel reports, for universities to create new structures to better serve research and education in computational science. Thus, we feel that although we are the first, we are not going to be the last and, in fact, we will be the model for how computational science is done at universities.

The missions of the Department are much the same as those of the SCS: to do world-class research in computational science, to offer innovative degree programs in computational science, and to support high performance computing on the FSU campus. The Department took over the Master's and Ph.D. degree programs already in place at the SCS and we are in the midst of the approval process for offering a B.S. degree program in computational science.

In this edition of the newsletter, we feature the 17 founding faculty members of the Department. The diversity in the backgrounds of the collective faculty stands out from even a cursory look at the brief descriptions given for each faculty member. A little closer inspection of those write ups shows what we have in common: an interest in the development and implementation of new algorithms for solving science problems using computers.

Future editions of the newsletter will feature our students and postdocs and our administrative and computer support staffs. We will also resume featuring the research and other activities of individual faculty and faculty groups.

These are very busy but also very exciting times for everyone associated with the Department of Scientific Computing. Of course, being the only one, we are the best such department in the nation. Our goal is nothing less than remaining the best, even later when there are dozens of similar departments!

The Faculty

PETER BEERLI and his group are interested in computational evolutionary biology, particularly population genetics, a field that builds the foundation for understanding the processes of evolution. Their research concentrates on the development of analytic methods and computer programs and their application to data from several species. Currently, the group's primary research focus concerns inferences of the amount of genetic interaction among populations and species. Some questions they might try to answer are: How well are populations of humans, humpback whales, or influenza viruses connected? How quickly does a particular species immigrate into a new area? What effect have population genetic model misspecifications had on our inferences? To help answer these

questions, the Beerli Group uses maximum likelihood and Bayesian inference to model population genetic interactions among individuals that are characterized by multiple genetic markers. From this data, they infer parameter values, such as population size and migration rates. These estimates advance their research and are helpful to other scientists working on projects like species conservation and modeling the spread of HIV or influenza in human populations. Beerli plans to extend these methods to allow estimation of population splitting or merging events and to study large numbers of genomic markers.

GORDON ERLEBACHER has a long history of multi-disciplinary research. His Ph.D. thesis studied new numerical techniques to solve free-boundary value problems in plasma physics using moving triangular meshes. Since then, his interests have ranged from the study of transition and turbulence in compressible flows using theoretical, symbolic and numerical methods, to the development of practical visualization algorithms for the scientist. Throughout this process, he has always strived to use the latest computational tools and techniques available.

Currently, Erlebacher is concentrating his efforts in four main areas. First, he is studying the properties and applications of the curvelet transform, which is a technique well suited to the capturing of curve singularities. In contrast, the very popular wavelet transform is well suited to the capture of point singularities. His group is applying the method to the separation of images into curve-like components and fuzzy point components using morphological component analysis, which seeks to minimize the number of terms in a basis expansion using multiple over-redundant dictionaries. Ultimately, they wish to analyze the structure of butterfly wings whose characteristics integrate both curve-like and point-like features. Second, he has recently become involved with the numerical complex geometry of the whale, particularly when the mouth is open and the whale is swimming. He and his group are interested in understanding and predicting whale swimming patterns. The third research area involves the use of graphical programming units (GPUs) for visualization and numerical computation. GPUs have, in the last three years, undergone a revolution and are now seen as much more powerful than the CPUs in our desktop computers

and notebooks. Professor Erlebacher and his group are investigating the use of GPUs to conduct finite-element calculations, Voronoi mesh generation, and the simulation of biological processes. The challenge is to harness these GPUs within the context of a computer cluster. Currently, they are running simulations on the 16-GPU cluster in the Mathematics Department. Finally, Professor Erlebacher is interested in the automation of web service generation in the context of information technology. Almost any task that is handled on a remote computer can be integrated within a web service. He and his lab members have written an application that takes scripts written in any of several languages and automatically transforms them into web-based applications with a graphical user interface with minimal user intervention. They expect this kind of tool will gain in popularity given the thousands of existing scripts.
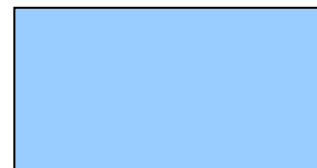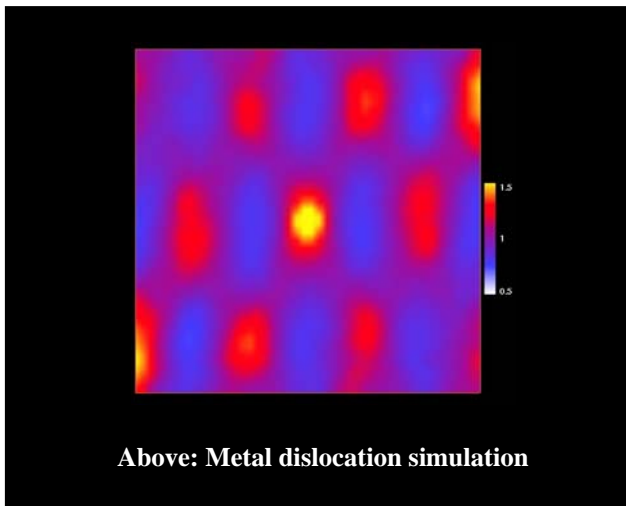
ANTER EL-AZAB is an Associate Professor of Computational Materials Science and Mechanics at the Department of Scientific Computing. He holds a Ph.D. in Nuclear Engineering from UCLA, and has worked with several research groups — including the Fusion Science Group at UCLA and the Computational Mechanics, Applied Mathematics, and Nanoscience Groups at Pacific Northwest National Laboratory — before joining Florida State University in Fall 2004. His research interests include mesoscale mechanics and metal deformation, radiation effects in materials, and thin films and coatings. He and his students develop theoretical models and computational techniques to understand the collective behavior of dislocations in metals, morphological stabilities in thin films, microstructure evolution and compositional changes in irradiated materials and structure of nanoscale materials systems. El-Azab has organized and co-organized many international workshops, symposia and conferences, including the Fourth International Conference on Multiscale Modeling of Materials in October 2008. He is a member of the Academic Executive Committee of the Materials Science Program at Florida State University.

MAX GUNZBURGER serves as the Frances Eppes Professor and Chair of the Department of Scientific Computing. The principal focus of his research is the invention, analysis, and implementation of computational algorithms and their application to diverse problems in science and engineering. His current algorithmic interests include numerical methods for partial differential equations (PDEs), especially finite element methods; control and optimization problems constrained by PDEs; computational geometry including grid generation; stochastic PDEs; and centroidal Voronoi tessellations. His current application interests include multiscale material modeling, ocean and ice flows, uncertainty quantification, groundwater flows in karst aquifers, image registration, superconductivity, turbulence, and finance. Over his career, Gunzburger has authored or co-authored six books and over 300 articles; has served as the advisor to 32 Ph.D. students, many of whom have gone on to have important research careers; has been funded by the NSF, DOE, DOC, DHS, AFOSR, ONR, ARO, and NASA; and has served as a consultant to two NASA, three DOE laboratories, and several companies. He has received several awards and honors, including the 2008 W.T. and Idelia Reid Prize in Mathematics awarded by the Society for Industrial and Applied Mathematics and a Guest Professorship at Peking University.

Above: Metal dislocation simulation

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and the Jet Propulsion Laboratory as well as previous academic positions at the University of Pittsburgh, Virginia Tech and Iowa State University. Professor Peterson is the current Associate Director for Graduate Studies in the Department of Scientific Computing. Her duties include managing the graduate degrees in computational science, recruiting new graduate students and mentoring current students as well as chairing the Curriculum and Admissions Committee.

TOMASZ PLEWA is an Associate Professor of Computational Astrophysics. His scientific interests include development and application of new algorithms for computational astrophysics and fluid dynamics. He works on developing high-performance parallel adaptive mesh refinement methods for large-scale multiphysics applications. He initiated this research in the Max Planck Institute for Astrophysics in Germany and, before moving to FSU, continued it while leading the Computational Physics and Validation group in the DoE ASC Alliance Center at the University of Chicago. Current development focuses around the Ardent package of high-order finite volume methods, multigrid solvers for elliptic and parabolic PDEs, and a radiative transport solver. Ardent is used to study violent and unstable fluid dynamics phenomena involving shockwaves, strong gravity, radiation, and thermonuclear reactions and transport of nuclear species. These physics components are essential in

modeling supernova events produced by massive stars and thermonuclear explosions of white dwarfs. Thermonuclear supernovae belong to the brightest objects in the Universe and play a central role in theoretical cosmology. Plewa is also an active participant in the High-Energy Density Laboratory Astrophysics, a community of researchers focused on reproducing extreme conditions found inside stars and in the interstellar medium in HEDP laboratories. Prime experimental facilities in these investigations are the Omega laser at the University of Rochester, Nike laser at the Naval Research Laboratory, and (soon) the LLNL National Ignition Facility (NIF).These interactions offer ideal settings for Verification and Validation (V&V) activities in computational science connecting basic science research into fluid instabilities and theoretical astrophysics with experiments.
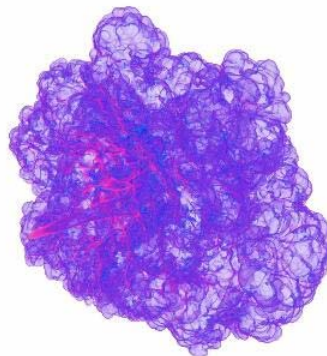
Volume rendering of an unstable flame front
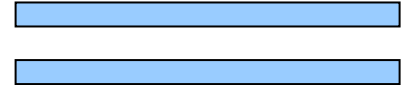
PROFESSOR SACHIN SHANBHAG is a chemical engineer who received his Ph.D. in polymer physics from the University of Michigan in 2004. During this time he used a combination of Monte Carlo simulations and mean-field theory to establish connections between the structure and rheological properties of so called "long-chain branched polymers" (which account for about 50% of all the polymers consumed, all the way from milk bottles to space-crafts). He spent a couple of years as a post-doc applying computational methods such as Brownian dynamics, quantum mechanics and cellular automata to study problems involving the self-organization of nanoscopic moieties, and in the design of a new class of ordered tissue engineering scaffolds. He joined the Department of Scientific Computing as an Assistant Professor in 2006, and currently works on the dynamics of ring polymers, crystallization of copolymers, and computational problems in nanomaterials.
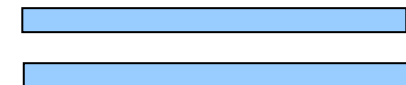
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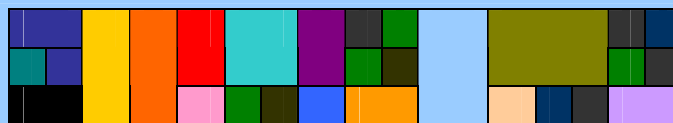
Research in **ALAN LEMMON**'s lab focuses on two exciting areas of computational evolutionary biology: speciation and phylogenetics. In the first area, the Lemmon group has

developed analytical models of the process of speciation as well as statistical models/methods for estimating key parameters of the speciation process. One current focus is statistical phylogeography, the study of the processes that produce genetic diversification within a species or group of closely related species. This work utilizes maximum likelihood and Bayesian statistical approaches to integrate data from diverse fields such as genetics, ecology, environmental niche model-ing, and geology into a unified spatially-explicit statistical framework. Lemmon's group has also worked extensively in the field of computational phylogenetics. One focus has been to develop and test complex statistical models used in phylogenetic reconstruction. Much of this work involves computationally

intensive simulations, and thorough phylogenetic analyses. The goal of this research is to ensure the methods used in phylogenetics produce accurate estimates of phylogeny and realistic estimates of uncertainty. A new focus of Alan's lab is to help prepare the field of phylogenetics for the enormous quantity of genetic data that the new genomics era will soon introduce. Particular areas of focus include large-scale marker development and high throughput phylogenetics in non-model systems.

ANKE MEYER-BAESE's research interests are in medical imaging, systems biology and informatics applied to structural and translational biology. In medical imaging, her research is focused on novel methods for pattern analysis, visualization and computer-aided diagnosis in the field MRI, such as functional MRI for human brain mapping, dynamic cerebral contrast-enhanced perfusion MRI and new approaches to breast cancer diagnosis in MRI mammography. She develops and applies novel combinatorial optimization and exploratory data analysis techniques in biochemical data analysis. She collaborates with the National High Magnetic Field
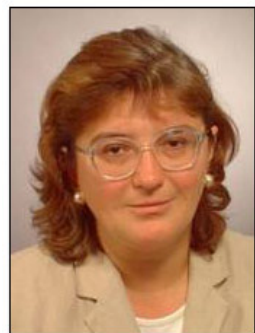

Laboratory, the Max Planck Institute for Informatics and the University of Jena in these areas. She published over 150 papers and is author of the book "Pattern Recognition in Medical Imaging" in Elsevier/Academic Press in 2003 and the forthcoming book "Biomedical Signal Processing: Advanced Methods and Applications" with MIT Press. Meyer-Baese is a recipient of the NIH Research Career Award, the Humboldt Research Fellowship and many others prizes and awards.

I. MICHAEL NAVON has a multidisciplinary educational background and research agenda encompassing physics, mathematics, and atmospheric science. His research focuses primarily on three areas: Advanced 4-D Var Data Assimilation Methods, Large Scale Minimization, and Ensemble Kalman filter methods. His research on the mathematical

theory of optimal control of partial differential equations for distributed parameter systems
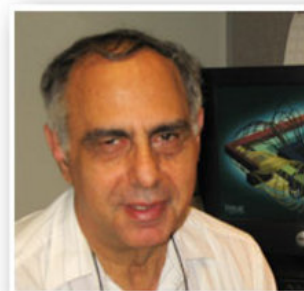
was for many years sponsored by the National Science Foundation and the National Aeronautics and Space Administration. Some of Professor Navon's most recent research focuses on partial differential equation constrained optimization in conjunction with multifaceted aspects of proper orthogonal decomposition model reduction linked to optimal control of fluids and applied to deficient 4-D VAR data assimilation methods. Much of his work on sequential methods for data assimilation applied to atmospheric models involving Ensemble Kalman filter, particle filters and maximum likelihood ensemble filters is pursued in collaboration with Professor Milija Zupanski and his group at Colorado State University.

Navon frequently collaborates with colleagues from all over the world. Among those collaborating with him in his research are staff from Imperial College (London), Academia Sinica (Taiwan), Energya Corporation (Russia), Virginia Tech and the University of Portland.
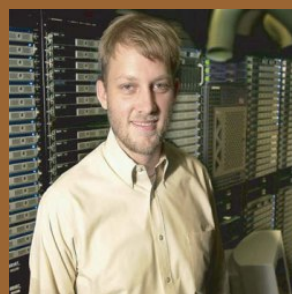
GAVIN NAYLOR is a biologist. He is interested in understanding how new traits arise over the course of evolution. This involves two lines of investigation: exploring the mappings between levels of organization in living architectures to shed light on how perturbations at low levels (mutations) have consequences for higher level features (proteins, cells, tissues organs) and (2) reconstructing the evolutionary path that shows which organisms gave rise to which. Naylor's group explores the

mappings between DNA sequence, amino acid and proteins. There is more variation at the level of DNA than there is at the level of amino acids due to the redundancy of the "genetic code" and considerably more variation at the level of amino acids than there is at the level of protein structure due to the redundancy of the "protein folding code". An explicit mapping of the inter-relationships and context

dependencies at these three levels should allow them to predict the effect of individual mutations on the form and function of the protein. They use phylogenetic analysis of DNA sequence comparisons to estimate the evolutionary relationships among different organisms. The lab is not restricted to any particular group, but a major project in the lab involves reconstructing the evolutionary tree for sharks and rays based on DNA sequence comparisons. They focused on sharks and rays because (1) they exhibit a diverse range of traits, and (2) they have an excellent fossil record that can provide a temporal component to our understanding of the origin of their novel traits. A diverse array of projects are currently underway in the Naylor Lab. They include: Molecular Phylogeny of Sharks and Rays, Mitogenomics of Elasmobranchs, Phylogeny and Population Genetics of Pristis, Protein Structure/Function Effects on DNA Sequences, Reconstructing Fossil Proteins, New Evolutionary Models for Mitochondrial Genome, Sequencing Hybridization and Morphometry of Protein Structure.

JANET PETERSON's active areas of research are numerical analysis and numerical methods for partial differential equations. She has investigated applications in areas as widely diverse as superconductivity and cancer cell growth. She has held positions at several national labs including Los Alamos National Laboratory, Sandia National Laboratory


Los Alamos National Laboratory, working on the application of enhanced sampling algorithms to study the folding of small proteins and their interaction with lipid membranes. In 2004, Nymeyer joined FSU's School of Computational Science and the Institute of Molecular Biophysics. The Nymeyer Laboratory is primarily interested in understanding how the structure of biological molecules leads to their functional properties. Ongoing projects include the simulation of small proteins to understand the chemical determinants of protein structure, folding mechanisms and rates; simulations of biological membranes to understand their physical properties; the development of simplified and coarse-grained models of biological membranes and proteins; and the development of codes to design new protein structures. Algorithm development forms a critical component of this research. New algorithms are being developed to extend the time and length scales that can be accessed with atomistic simulation. They provide
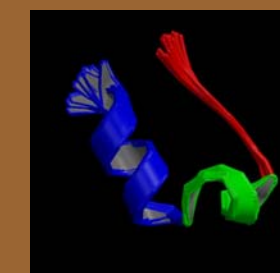

LEFT: PROTEIN FOLDING IMAGE FROM THE NYMEYER LAB

improvements in sampling efficiency of several orders of magnitude beyond existing techniques.

DENNIS SLICE works on Morphometrics, the development and application of tools for biological shape analysis. This includes addressing problems associated with the acquisition, processing, and analysis of variables related to shape - the geometric properties of an object invariant to location, orientation, and scaling. Whereas traditional approaches in this field focused on linear and angular measurements to capture shape information, newer methods work with configurations of anatomical points (landmarks) whose relative locations are encoded in their Cartesian coordinates. The analysis of data from either approach is essentially the same, but coordinate-based methods require different handling prior to analysis. In return, they provide a more comprehensive description of shape that can be used to generate meaningful and compelling visualizations of statistical results not possible with more traditional data sets. The potential of such methods is extensive as they are useful in every area of organismal biology. Some specific projects with which Slice is involved include the development of software to characterize human crania (with N. C. State and the National Institute of Justice), assessing the components of facial variation related to respirator fit/function (CDC/NIOSH), and quantifying aspects of car fronts associated with their perceived personality traits (University of Vienna and EFS Unternehmensberatung GmbH, an auto-design consultancy).
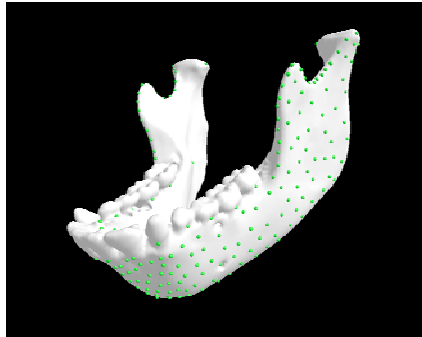
Chimpanzee mandible showing system of landmarks used to quantify growth and development.
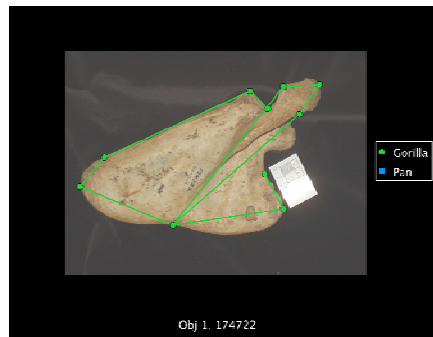
Gorilla scapula with marked anatomical landmarks used to study biomechanics of locomotion in apes
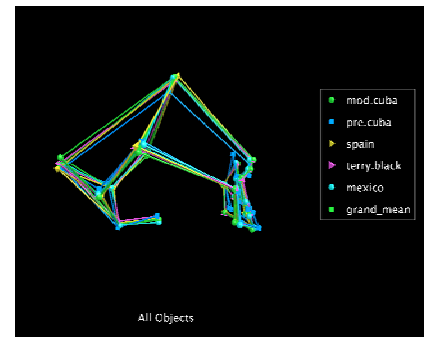
Principal components summarizing mult-variate variation in the leaf morphology of different species of Italian oak trees.

XIAOQIANG WANG was a software engineer before graduating from Pennsylvania State University in 2005, and now focuses his research on using numerical analysis and applied partial differential equations. His industry experience informs his research focus in applying computational science to solve industry problems. His research interests include numerical analysis and applied partial differential equations, mathematical biology, image processing, scientific visualization, data mining and high-performance scientific computing. At present, he devotes himself to the research and numerical simulation of biological cell membranes.

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JAMES WILGENBUSCH is a Research Associate in the Department of Scientific Computing, Director of Florida State University's High Performance Computing facility and supervisor of the Technical Support Group in the Department of Scientific Computing. In addi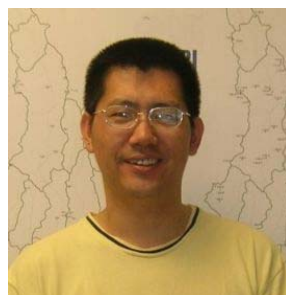tion to his administrative responsibilities, James also maintains an active research program in the study and implementation of models and search algorithms used in Bayesian and likelihood-based phylogenetic inference. Results from his work are published in such journals as Bioinformatics, Current Protocols in Bioinformatics, and Systematic Biology and have also been presented at numerous scientific conferences and annual meetings. James is also regularly invited to be involved in activities beyond FSU's campus. These outreach activities include serving on review panels for the National Science Foundation (e.g., TeraGrid Annual Review; High-Performance Computing for Science and Engineering and Education: Operations; Biological Databases and Informatics; as well other ad hoc reviews), serving as an editorial board member for Systematic Biology, and teaching in workshops around the globe (e.g., Recent Advances in Conservation Genetics sponsored by the American Genetic Association, Laboratory of Genomic Diversity/National Cancer Institute, Front Royal, Virginia and Oahu, Hawaii; Introduction to Phylogenetic Inference, Department of Biochemistry, Srinakharinwirot University, Bangkok, Thailand; Principles and Methods in Phylogenetic Analyses,

National University, La Plata, Argentina). Prior to coming to FSU in 2001, James worked at the Smithsonian Institution's Laboratory of Molecular Systematics. At the Smithsonian, James employed molecular techniques to obtain DNA sequences and implemented novel analytical methods to infer the evolutionary history of diverse and widespread biological organisms.

MING YE's research area is computational hydrology/geology, with a focus on groundwater flow and contaminant transport modeling. His research involves quantifying and reducing uncertainty in predictions of groundwater flow and contaminant transport. The predictive uncertainty is an important criterion used for decision-making in many environmental issues. Supported by the Nuclear Regulatory Commission and Department of Energy, Ye has completed several projects that simulate radionuclide transport in various geologic media. A recent application of his modeling expertise is for a former experimental atomic area in Rulison, Colorado, an underground area irradiated in the 1970s when an atomic bomb was tested as a means of fracturing rock to release trapped gas for production. Whereas natural gas resources at the site are worth 200 Million dollars, gas production is hampered due to potential transport of tritium from the former test. His modeling shows that risk at the site is low, by simulating the movement of tritium in both water and natural gas. Ye is mentoring one masters student and two doctoral students in Scientific Computing and Geology.

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