The FSU School of
Computational Science
& Information Technology

COMPUTATIONAL Xposition 2004

CSIT GRADUATE STUDENT PRESENTATIONS

Welcome to Computational Xposition 2004

Computational Science is an emerging discipline that uses advances in mathematics and computer science to simulate complicated, real-world processes such as how proteins fold, how hurricanes move, or how wildfires spread. Understanding these processes requires a multi-faceted approach – observations, experiments, and theory – whose elements are synthesized in computer simulations and computations. Computational Scientists include the people developing new approaches and techniques in the mathematical sciences and the people applying those advances in the natural, social, and engineering sciences.

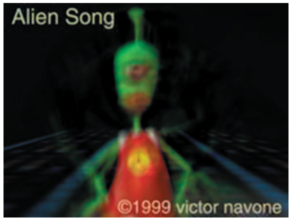
As the problems and methods suggest, Computational Scientists can be found in a wide range of disciplines and students are being trained in Computational Science in an ever-increasing range of departments. Students working in Computational Science are drawing upon, and mastering, ideas and methods from a diversity of traditional disciplines. These are not easy intellectual roads to walk; but in doing so, these students are defining new ways to answer difficult questions. And as they succeed, they are shaping our ideas about how to train the next generation.

We are glad you can join us to celebrate the continued evolution of Computational Science and the evolution in the training of Computational Scientists. We hope you find the students' work exciting and that their enthusiasm and energy shines through their posters and demonstrations.

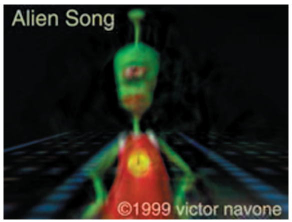
Joe Travis
Director, CSIT

Christopher G. Baker
MS Computer Science

A Block Incremental Algorithm for Computing Dominant Singular Subspaces



Subspace tracking is utilized in almost every computational discipline. Many problems in signal processing, statistics, computer vision, and engineering are formulated in the context of large dimensional spaces. Computing in these scenarios is often not feasible. This can be resolved by projecting the system onto a smaller dimensional space. This idea gives rise to such methods as the Fisher Linear Discriminant, Principal Orthogonal Decomposition, and many other techniques.

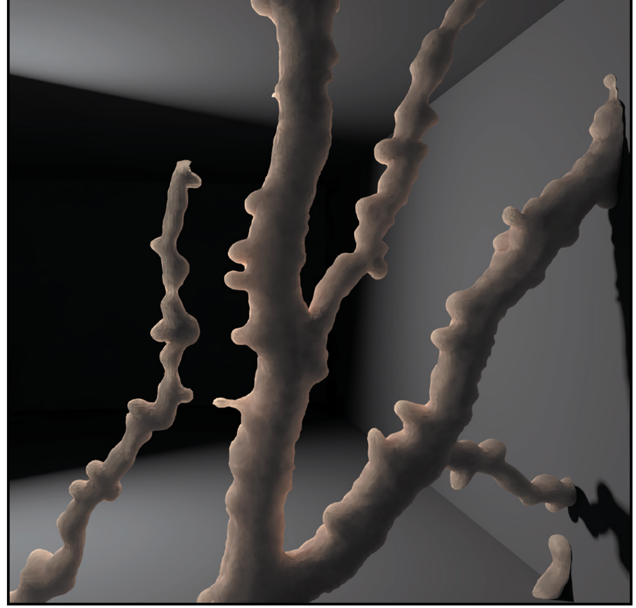


The scope of my research involves many topics in this area. My Masters Thesis outlined an algorithm for incrementally computing approximations to the dominant singular subspaces of a matrix. My research with, among others, Y. Chahlaoui explores numerous methods for computing optimal projectors for model reduction of large, sparse dynamical second-order systems. Finally, ongoing research with P.-A. Absil and K. Gallivan explores trust region methods on Riemannian manifolds, with applications in computing optimal spaces for numerical linear algebra and other areas.

Courses taken outside of major

CIS 5930 Numerical Linear Algebra I
CIS 5930 Numerical Linear Algebra II
STA 5106 Computational Methods in Statistics I
STA 5107 Computational Methods in Statistics II
MAT 5933 Quantum Computing

Kevin Beason
MS Computer Science



Global Illumination of Isosurfaces

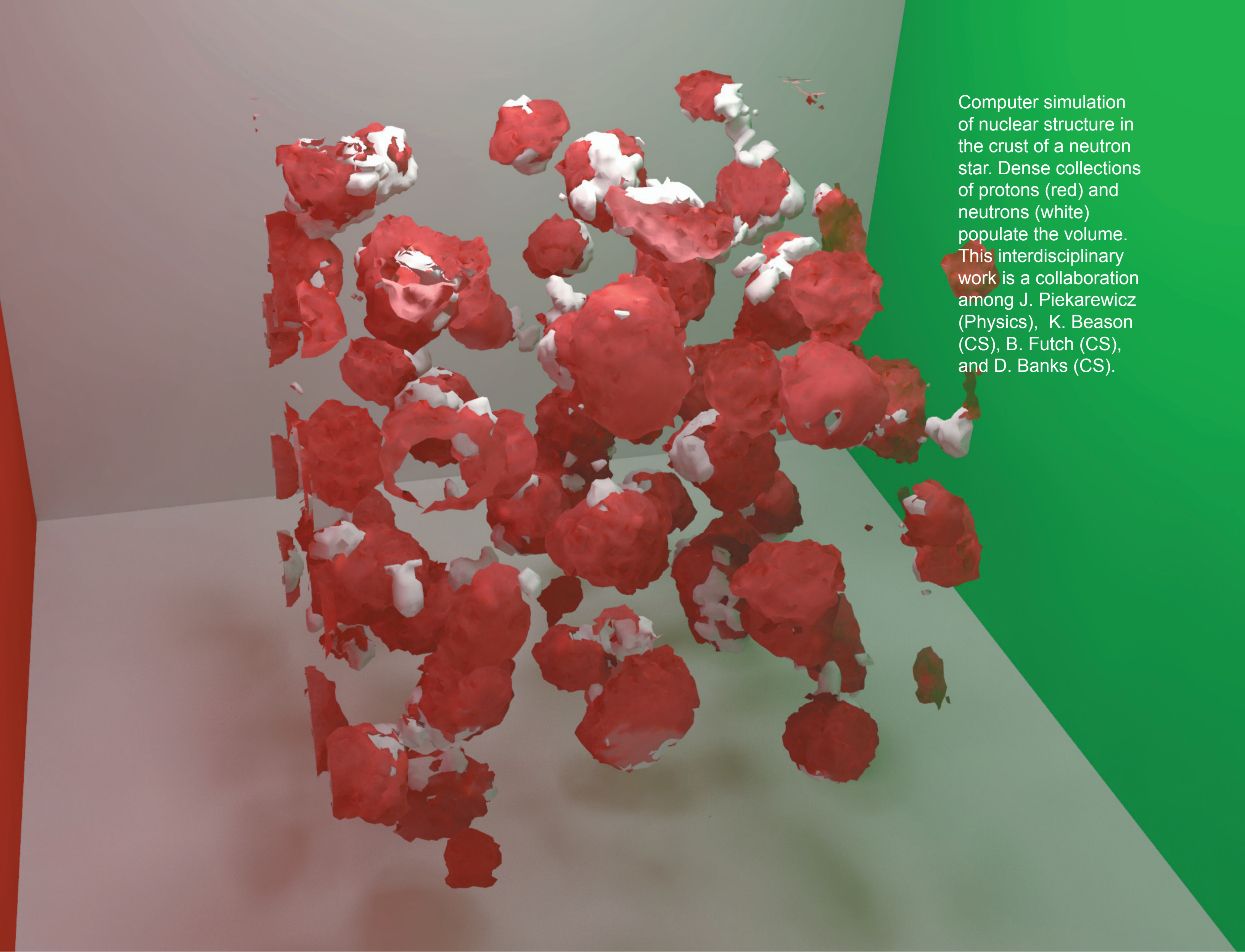
The purpose of my research is to upgrade the quality of 3D scientific visualization by applying global illumination to isosurfaces.

An isosurface of a three-dimensional (3D) function is a surface in which all the points have an identical value, called the isovalue. This isosurface may capture the shape of the brain (from MRI data), or of a nerve cell (from laser microscopy) or of neutron clusters (from a computational simulation of neutron stars). Often the shape is very complex, in which case the subtle effects of realistic lighting (like soft shadows, inter-reflection, and caustics) make the 3D structure more evident to the scientific user.

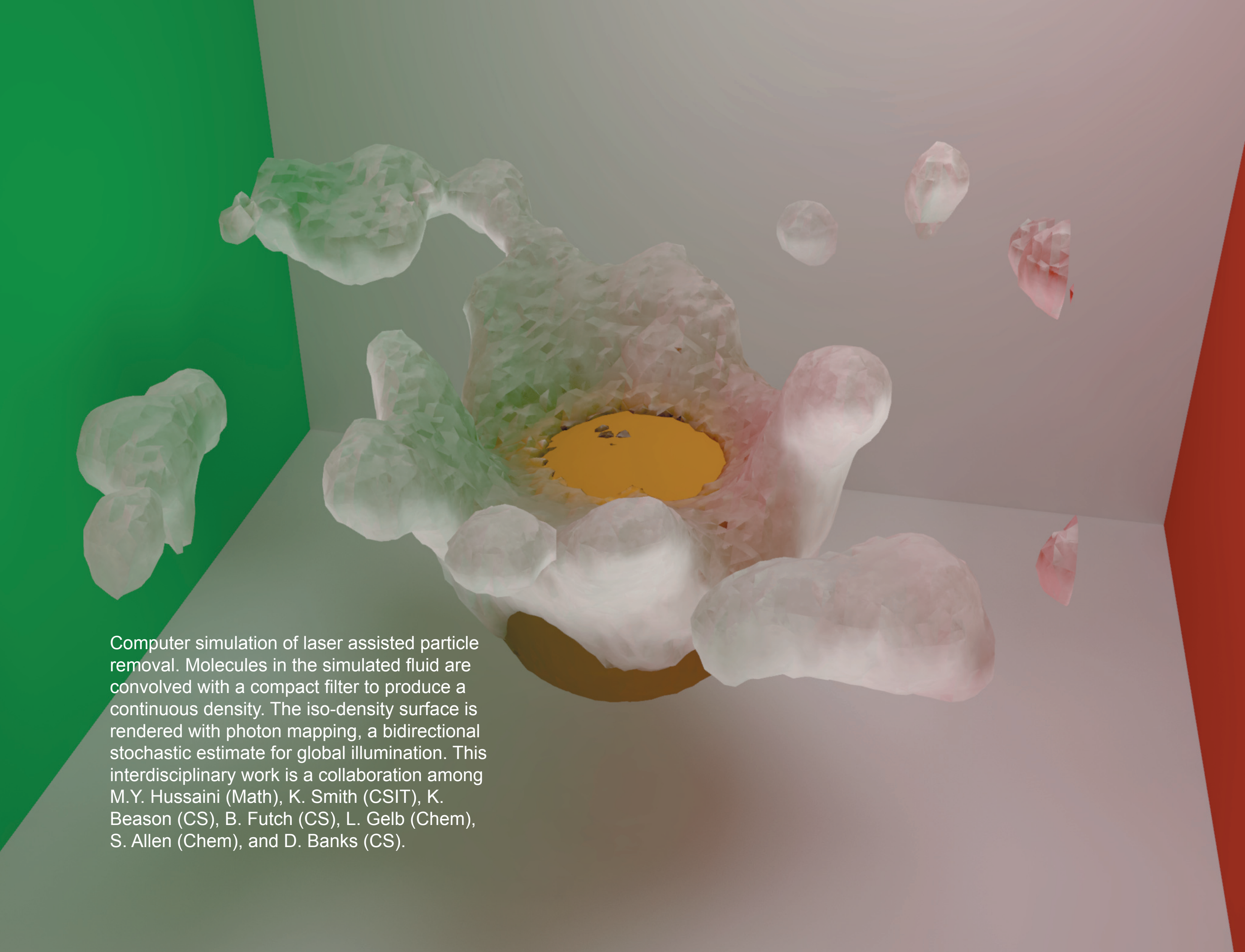
Unfortunately, solving the light-transport equation for these complex surfaces may take hours to complete. My work is the first to demonstrate that pre-processing allows these high-quality renderings to be produced using the video card of an ordinary home computer, and at the same speed as the low-quality "local illumination" provided by existing commercial tools for 3D visualization.

Courses taken outside of major

STA 5106 Computational Methods in Statistics I
STA 5107 Computational Methods in Statistics II
PHY 3424 Optics
ART 2010 Photography



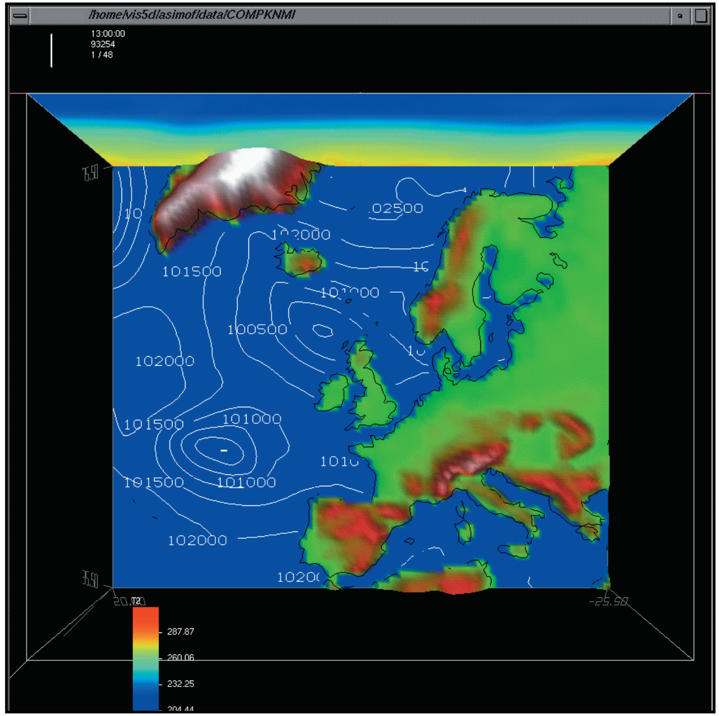
Computer simulation of nuclear structure in the crust of a neutron star. Dense collections of protons (red) and neutrons (white) populate the volume. This interdisciplinary work is a collaboration among J. Piekarewicz (Physics), K. Beason (CS), B. Futch (CS), and D. Banks (CS).



Computer simulation of laser assisted particle removal. Molecules in the simulated fluid are convolved with a compact filter to produce a continuous density. The iso-density surface is rendered with photon mapping, a bidirectional stochastic estimate for global illumination. This interdisciplinary work is a collaboration among M.Y. Hussaini (Math), K. Smith (CSIT), K. Beason (CS), B. Futch (CS), L. Gelb (Chem), S. Allen (Chem), and D. Banks (CS).

Arthi Gokarn
MS Computer Science

Internet computing with MATLAB



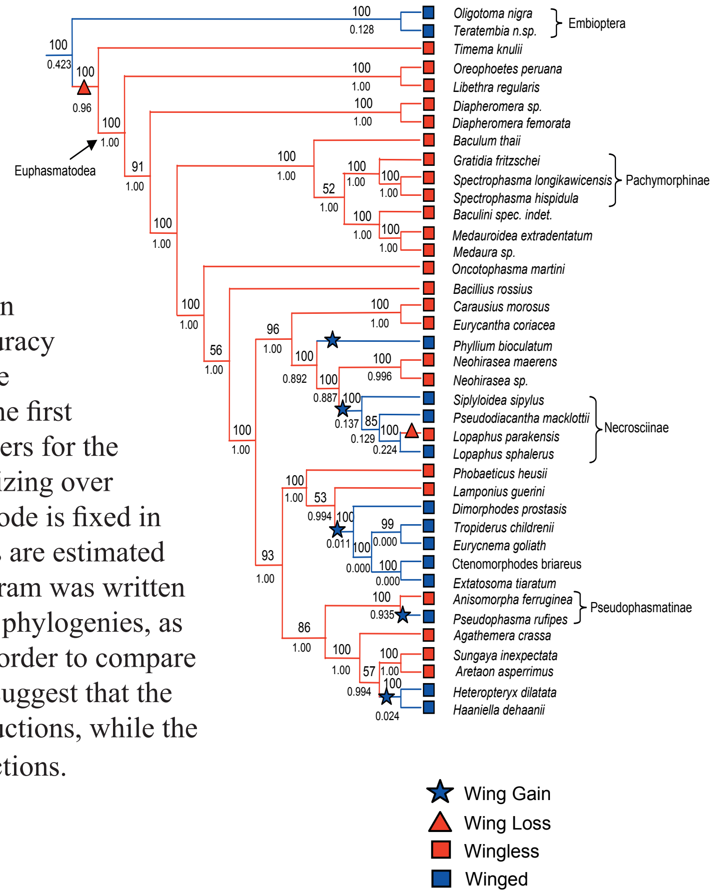
The purpose of this project is to create MATLAB® applications that use the capabilities of the World Wide Web to send data to a remote server for computation and to display the results in on a local MATLAB application. The data is sent to and received from the remote application using gSOAP.

Data can be sent to a remote server, which need not have a copy of MATLAB installed. This is accomplished by calling gSOAP functions from MEX-files written in the C programming language. The MEX interface code and accompanying C code is automatically generated by gSOAP. The use of the gSOAP compiler (which is part of this project) simplifies this task, which otherwise requires users to program most of the data communications at a lower level. This project specializes on efficient data representations for communication with Web services, such as sparse numerical matrix representations. The diagram shows the visualization of weather forecast data through MATLAB.

Vanessa Jackson
MS Biology

Maximum Likelihood Reconstruction of Discrete Ancestral Character States

Maximum likelihood methods are commonly used to reconstruct ancestral character states on a phylogeny in order to test hypotheses about evolution and adaptation. My thesis project examines the accuracy of two maximum likelihood variants used to estimate discrete characters states on evolutionary trees. In the first method, termed "global", the transition-rate parameters for the likelihood model are estimated only once by maximizing over all states. In the second method, termed "local", a node is fixed in a certain state and then the transition rate parameters are estimated conditional upon that state. A custom software program was written to perform reconstructions on a variety of simulated phylogenies, as well as phylogenies of real biological organisms, in order to compare the accuracy of these methods. Preliminary results suggest that the global method performs better on marginal reconstructions, while the local method may perform better for joint reconstructions.



Courses taken outside of major

MAT5932 Computational Biology
STA5107 Computational Methods in Statistics II

Hui Song
MS Computer Science

Face Recognition via Image Synthesis

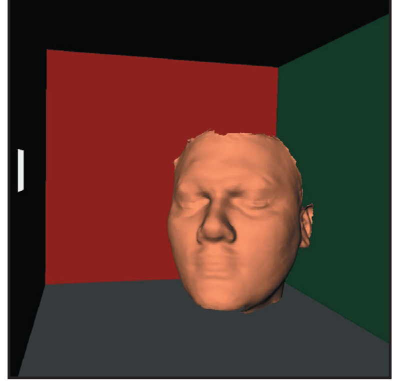
My goal is to automatically recognize a face in a photograph or in a video frame. To do this, I first generate an image (using 3D computer graphics) that matches a photographic image.

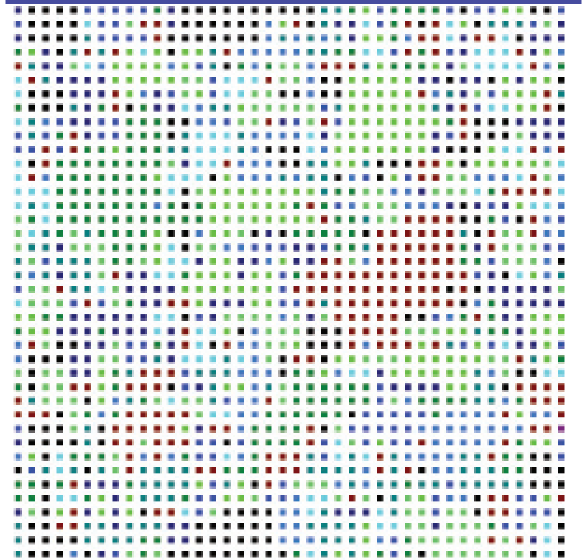
I use 3D laser scanner to capture the surface geometry of a face. Then I photograph the face from different directions and under different lighting conditions. I project a white disk onto CSIT's 8-foot by 16-foot Power Wall as the light source, then synchronize the shutter on a camera with the light source via network. The direction of the light and the direction of the view are all that are needed to reconstruct the reflectance function at points on the face.

I cluster the reflectance functions to match just a few basic regions of the face (such as lips, cheeks, forehead). Then I apply these clustered reflectances to the polygonal mesh, apply photon mapping with subsurface scattering, and generate the realistic 3D image. This is compared to the photograph for a possible match.

Courses taken outside of major

STA 5106 Computational Methods in Statistics I
STA 5107 Computational Methods in Statistics II





Alexander Velytsky
PhD Physics

A Model Study of the Deconfining Phase Transition

The study of the deconfining phase transition or crossover is important for the understanding of properties of nuclear matter and the quark gluon plasma. Heavy ion collisions experiments are capable of creating conditions necessary for deconfinement. The dynamics of this process and not only its equilibrium properties are of interest. In this project non-equilibrium aspects of rapid heating and cooling of the QCD vacuum are studied in a model framework. The 3-D Potts model with an external magnetic field is an effective model of QCD. It is studied by means of Monte Carlo simulations. Other models are used to understand the influence of the strength of the phase transition. In our investigations these systems are temperature driven through a phase transition or a rapid crossover using updating procedures in the Glauber universality class. We study hysteresis cycles with different updating speeds and quench simulations. Qualitatively this should reveal the physics of non-equilibrium configurations. A number of observables is measured during the simulations: Thermodynamical quantities such as the internal energy and the magnetization, properties of Fortuin-Kasteleyn clusters and structure functions. Comparing with equilibrium data we conclude that the Monte Carlo dynamics is capable of creating a spinodal decomposition, which dominates the statistical properties of configurations. A slowing down of the equilibration in the ordered phase due to the competition of different magnetization domains is observed. This could lead to a situation where the system does not fully equilibrize in the available time. Spinodal decomposition of the Polyakov loops may lead to an enhancement of low momentum degrees of freedom. If this scenario is realized by Nature, this may be observed in experiments as an increase in the low energy gluon production.