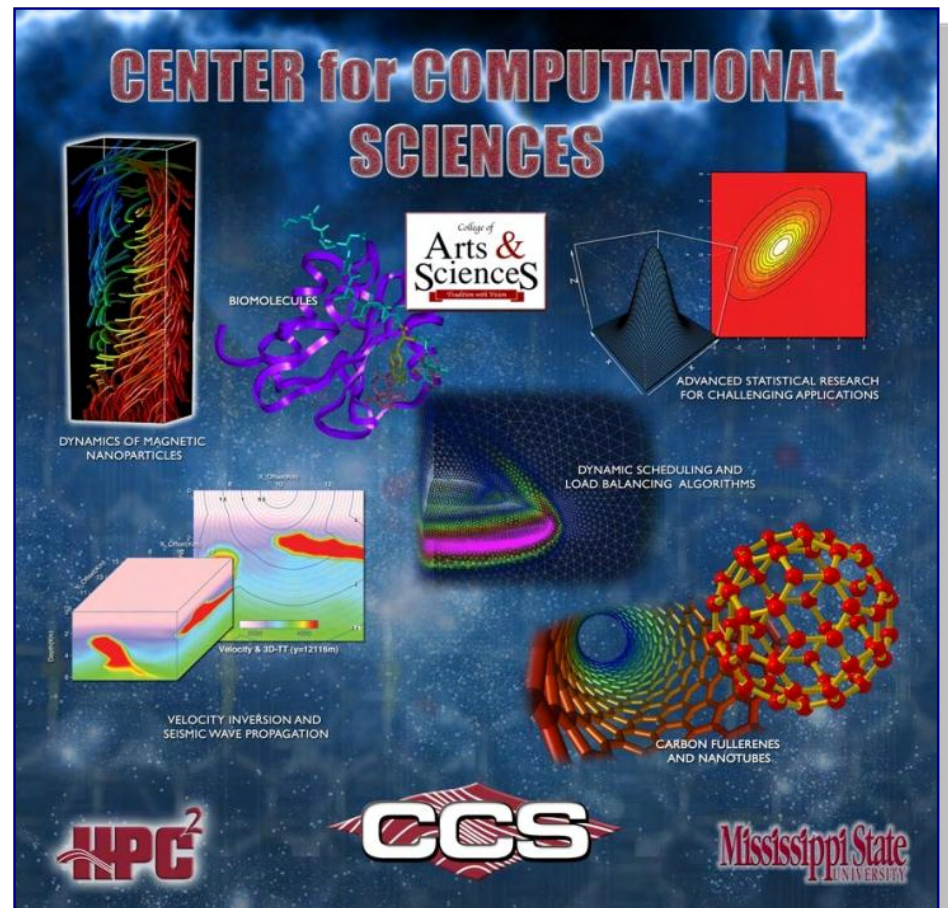


Center for Computational Sciences



Mission

To foster interdisciplinary in both the fundamental understanding and application of all the natural sciences. In particular, to model and develop integrated computational environments and crosscutting tools that allow a comprehensive, cross-disciplinary approach to problem –solving.



Computational and Applied Mathematics at CCS

Image Processing

- Image Denoising: Non-standard anisotropic diffusion (NSAD) model for edge-preserving noise removal:

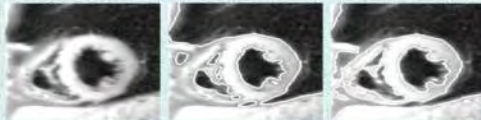


Original image (left), restored image using conventional model (middle), and NSAD (right)

- Image Segmentation: Method of background subtraction (MBS) for medical image segmentation:



Left: segmentation without MBS, right: MBS segmentation



Left: Original medical image, middle: segmentation without MBS, right: MBS segmentation

Population Dynamics

$$\frac{\partial u}{\partial t} = d\Delta u + u f(x, u) - c(x)h(x), \quad x \in \Omega;$$

$$u(t, x) = 0 \text{ or } \frac{\partial u}{\partial n}(t, x) = 0, \quad x \in \partial\Omega;$$

$$u(0, x) = u_0(x), \quad x \in \Omega, \quad t > 0.$$

'No place for fish to hide'

Damage to large species might be permanent

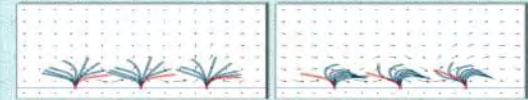


Popular species on decline in 13 fisheries analyzed

...and the loss of large fish could have a cascading effect on the entire ecosystem. The study, published in the journal *Science*, found that the number of large fish in 13 fisheries has declined by an average of 35 percent since 1970. The researchers say that the loss of large fish could have a cascading effect on the entire ecosystem, as they are often the top predators in the food chain. The study also found that the loss of large fish could lead to a decline in the number of smaller fish, as they are often preyed upon by the larger fish. The researchers say that the loss of large fish could have a cascading effect on the entire ecosystem, as they are often the top predators in the food chain. The study also found that the loss of large fish could lead to a decline in the number of smaller fish, as they are often preyed upon by the larger fish.

USA TODAY Article - Thursday, May 15 2003, 11D

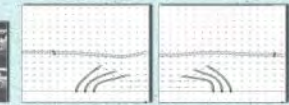
Computational Math-biology



Overlay of cilia geometry during recovery stroke and power stroke [Yang, Dillon and Fauci, An Integrative Computational Model of Multiciliary Beating, Bull. Math. Biol., 70(4):1192-1215, 2008]

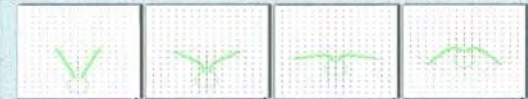


a) Ciliary activity of cultured rabbit tracheal epithelium: beat pattern and metachrony [Sanderson & Sleight, Journal of Cell Science, 47:1, 1981.]



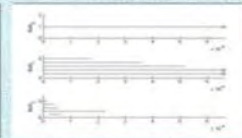
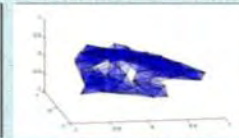
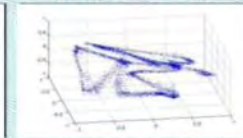
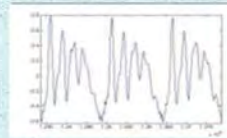
b) Our numerical simulations in Newtonian fluid [Dillon, Fauci, Omoto & Yang, Annals of the NY Academy of Sciences, 1101, 2007].

Mucociliary transport: experiment and numerical results.



Chlamydomonas is a genus of unicellular green algae used as a model organism for research on many fundamental questions in cell and molecular biology. One of the most interested questions is how the cell moves by the hair-like biflagella? The above pictures are the snapshots of the numerical simulation of the swimming of chlamydomonas using the internal force generation mechanism [Dillon & Fauci, 2000] in viscous, incompressible fluid.

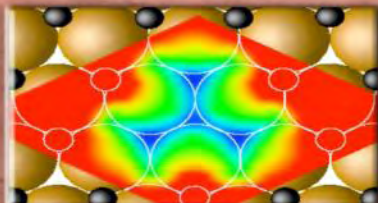
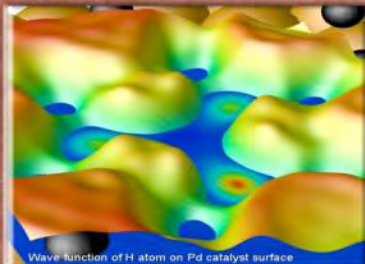
Topological Data Analysis



- Algebraic topology may be used to study point cloud data sets – a signal is embedded into three dimensions, triangulated, and its homology computed.

Computational Physics at CCS

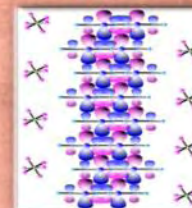
Quantum simulation of Hydrogen Catalysis



Micromagnetic simulation of nanomagnets



Quantum Monte-Carlo Simulation of Organic Superconductors



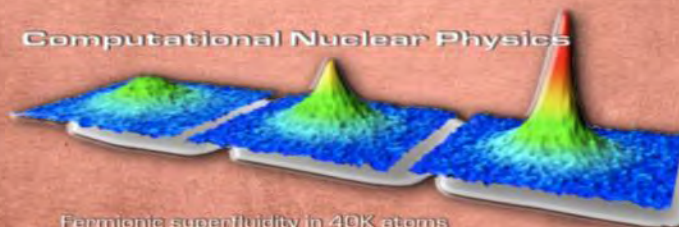
Atomistic Simulation of Nanopowder



Sintering of two nickel microparticles (experiment) and two tungsten nanoparticles (simulation)



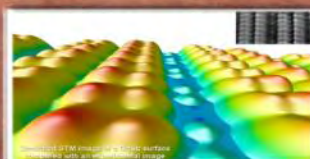
Computational Nuclear Physics



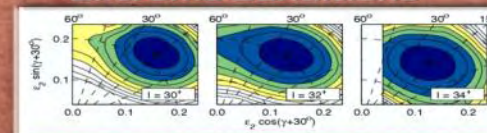
Nano-scale quantum mechanical simulations



Melting simulation of a C60 fullerene



Behavior of Nuclei at Extreme Conditions



Potential energy surfaces for the 74Kr ground-state band configuration



Computational Ecology and Evolutionary Biology at CCS

$$\frac{dI}{dt} = \beta SI - (\gamma + \phi)I$$

Mathematical
Epidemiology

Population Genetics
and Ecological Genomics

Molecular
Systematics

HPC²

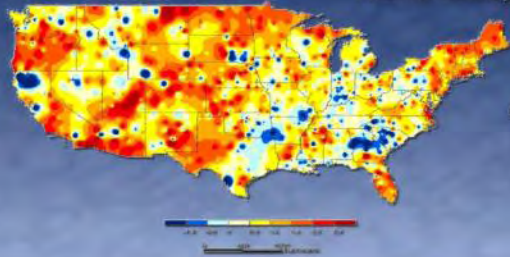
CCS

College of
Arts &
Sciences

Mississippi State
UNIVERSITY

Computational Statistics at CCS

Trend Study in a Periodic Time Series Regression Model



Annual temperature trend estimates in USA (left) and its spatially smoothed trend estimates (right).



Statistical Estimation Based on Censored Data
 (Hao-Guang)
 Department of Mathematics and Statistics
 Mississippi State University

In biometry, reliability, and medical follow-up studies, incomplete data are frequently encountered. One example is the case of censored data. We consider estimation problems based on censored data, such as the estimation of survival function, linear parameter, and non-parametric regression functions.

MLE of the Survival Function with Doubly Censored Data

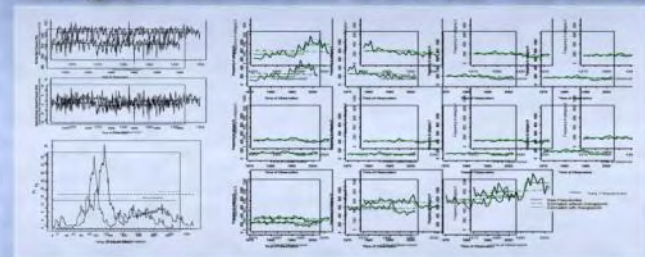
Non-consistency Estimation for Doubly Censored Data

$$F(x) = \int_0^x f(t) dt = \int_0^x \frac{1}{F(t)} f(t) dt$$

The MLE for the Survival Function with Doubly Censored Data

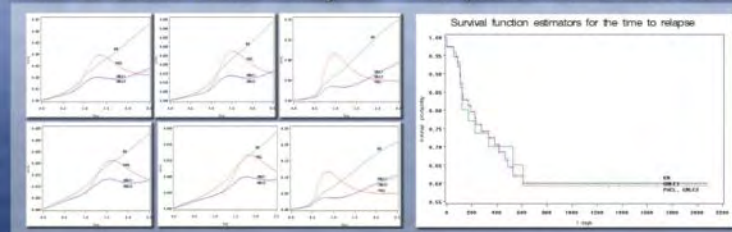
$$\hat{F}(x) = \prod_{i=1}^n (1 - \frac{d_i}{n_i - r_i})^{I(x \leq t_i)}$$

Changepoint Detection of Climate Time Series

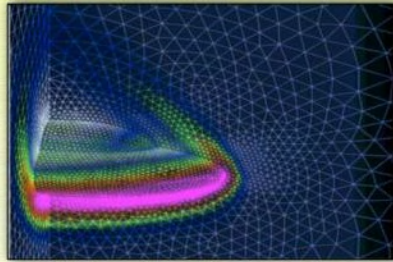


Changepoint detection for a monthly mean atmospheric pressure series (left) and a yearly frequency of cloudiness (right).

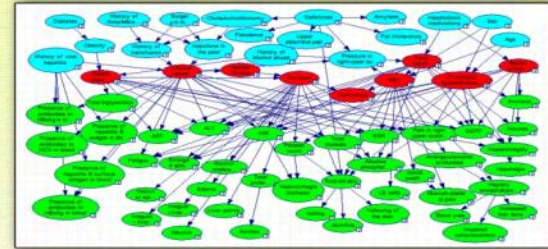
Time to Event Data Analysis – Nonparametric Estimation



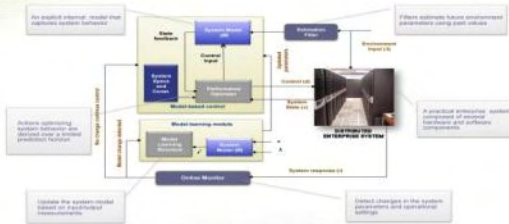
Modeling, Visualization and Optimization at CCS



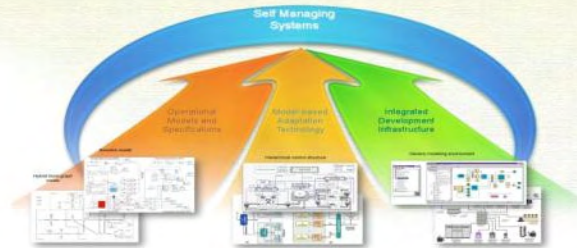
Performance Optimization of Problems in Computational Science And Engineering



Multiple-fault Diagnosis Using Bayesian Networks



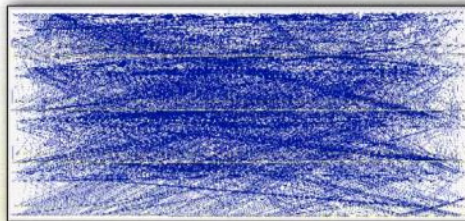
Control-based Framework for Self-managing Systems



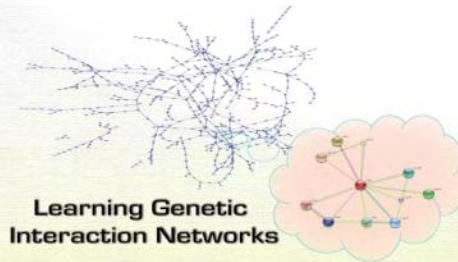
Model-based Self-managing Systems



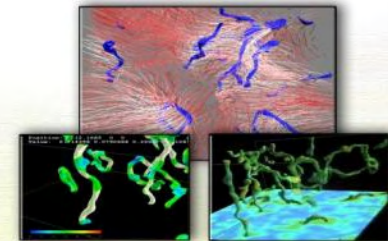
Modeling and Visualizing Neural Fiber Structures



Efficient Inference in Bayesian Networks



Learning Genetic Interaction Networks



Visualizing Nematic Liquid Crystal Defects

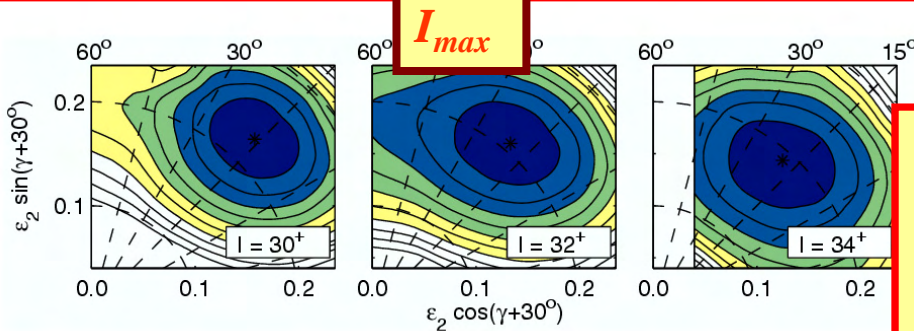
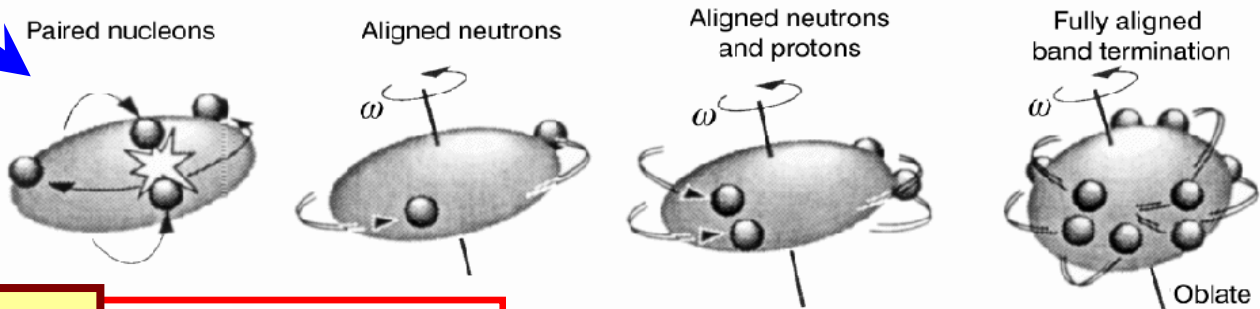


Anatoli Afanasjev (Dept. of Physics and Astronomy)

1. Extreme conditions in nuclei

Goal: to understand the behavior of nuclei at extreme conditions of fast rotation and/or large deformation and their pairing properties

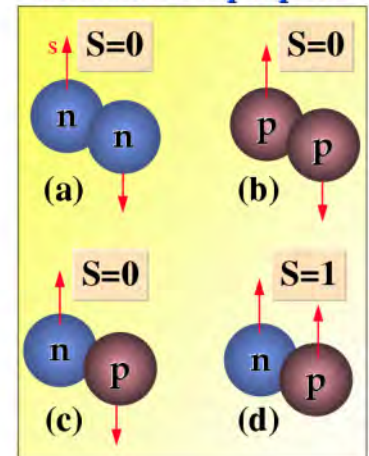
Termination and non-termination of rotational bands



Potential energy surfaces for the ^{74}Kr GSB configuration

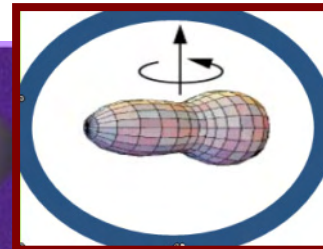
Proton-neutron pairing in N~Z nuclei

nucleonic Cooper pairs



Superdeformation and search for hyperdeformation

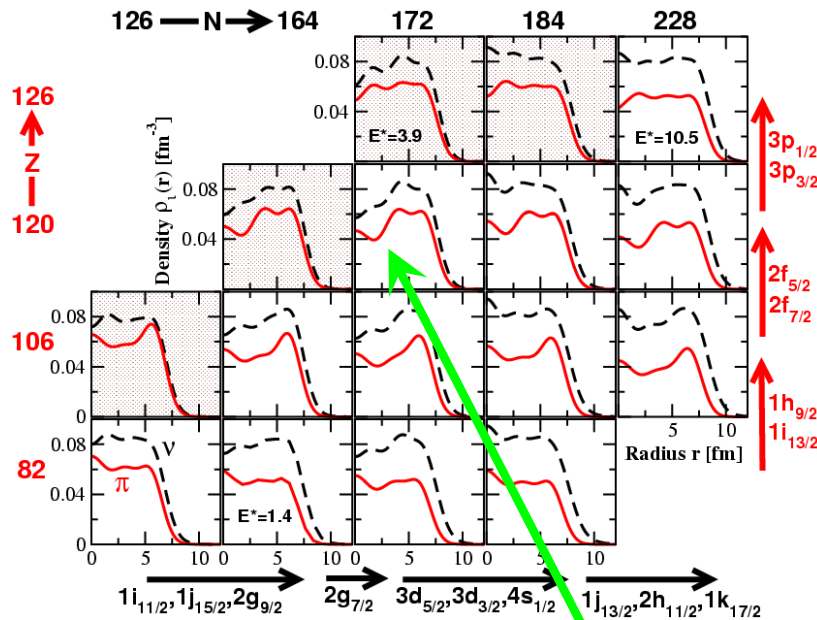
Nuclear Shapes



Anatoli Afanasjev (slide 2)

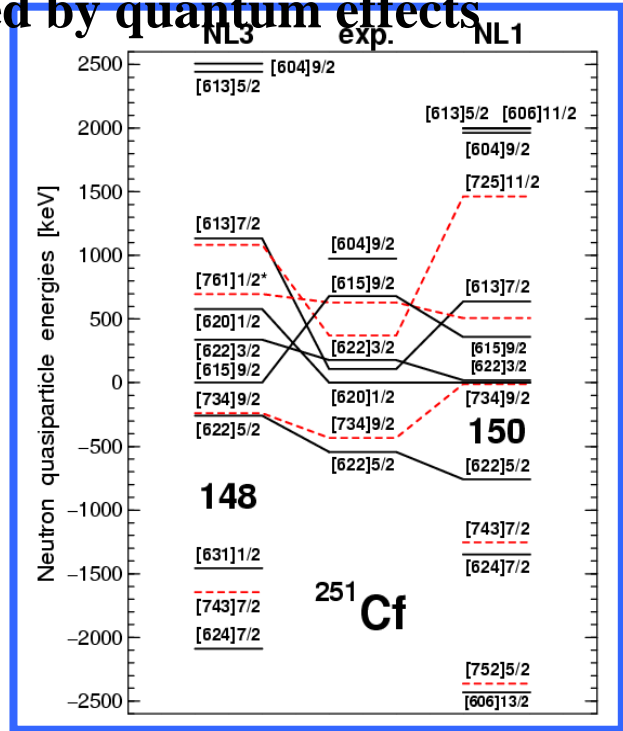
2. Physics of superheavy nuclei

Goal: to understand and predict the properties of superheavy nuclei – only nuclear systems completely stabilized by quantum effects



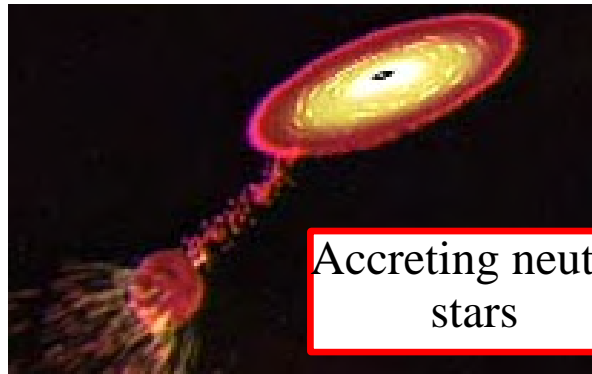
Densities of superheavy nuclei:
spherical relativistic mean field
calculations

*Central depression
in density distribution*

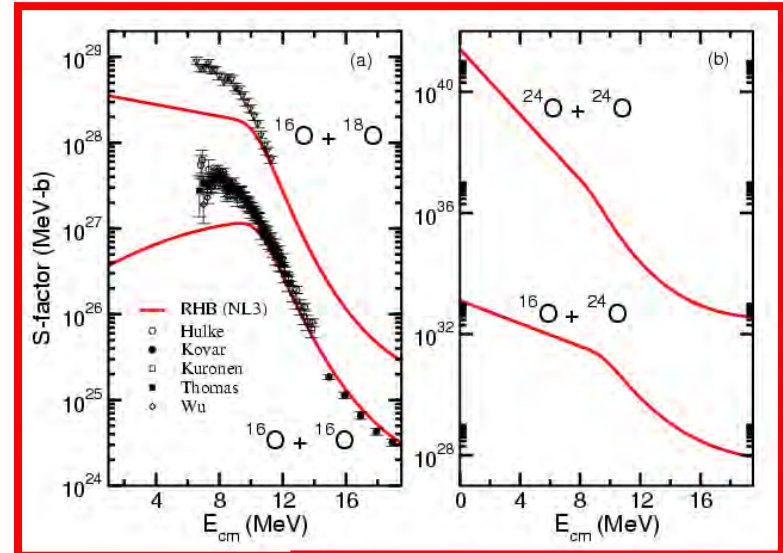
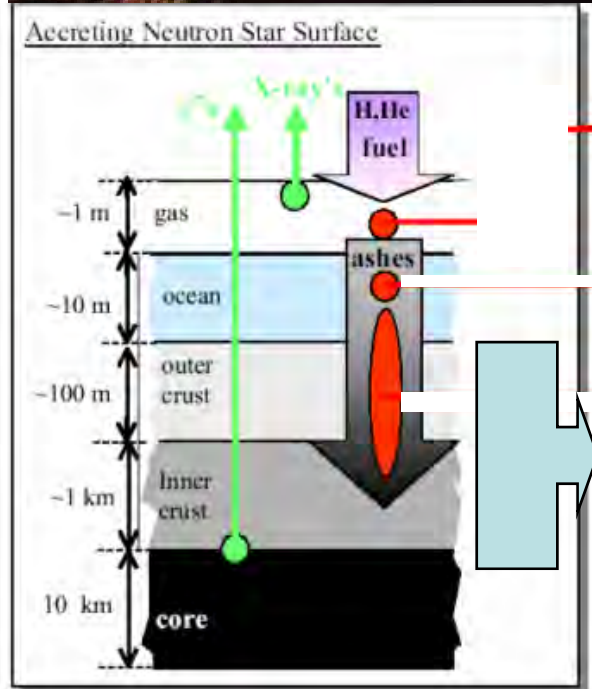


Building the gateway to superheavy
nuclei by studying single-particle
spectra and other properties
of heaviest actinide nuclei

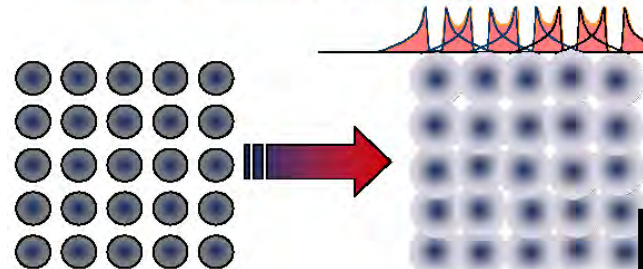
Goal: to understand pycnonuclear reactions in the crust of neutron stars and in dwarf stars; to derive their chemical composition.



Accreting neutron stars



Thermal & electrical properties of crust matter?

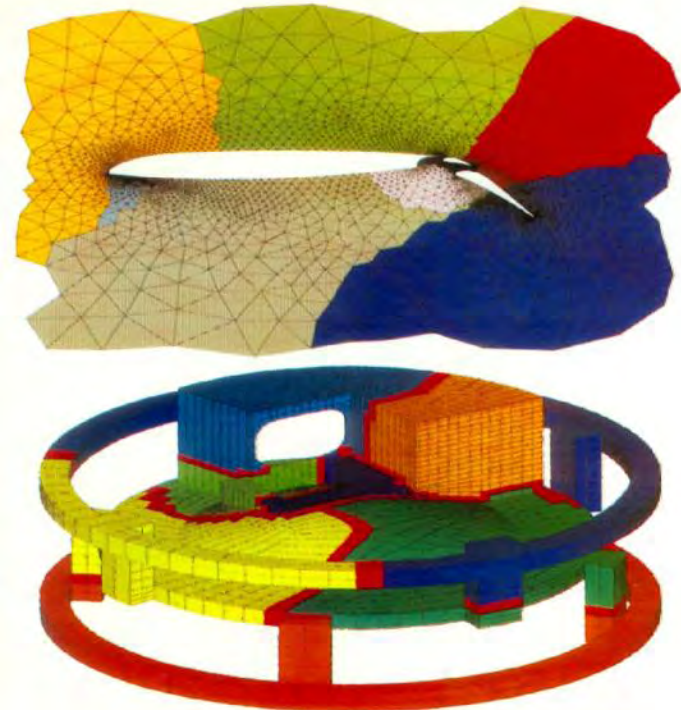
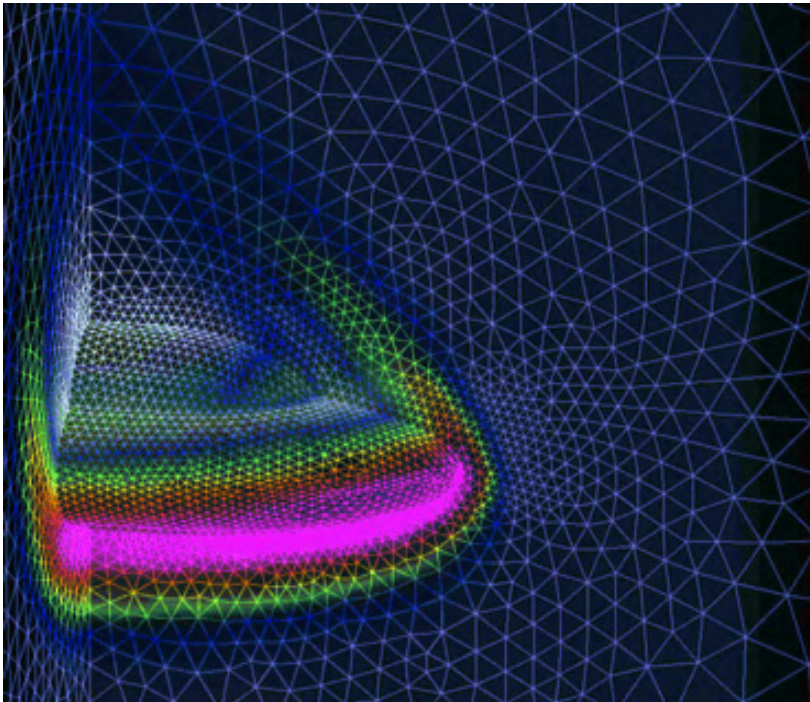


Compact lattice of nuclei + plasma screening = fusion (pycnonuclear) reactions at low $T \sim$ hundreds keV

The rate of pycnonuclear reactions is increased in neutron-rich nuclei

Generation of heat in deep neutron star crust through pycnonuclear reactions

Performance Optimization of Problems in Computational Science And Engineering



- **Goal:** to advance the state-of-the-art in dynamic scheduling and load balancing algorithms for improving the scalability and performance of parallel applications in scientific computing
- **Focus:** on the development of algorithms, techniques and tools that address load imbalance factors generated by the unpredictable behavior of simulations, such as irregularities rising from problem characteristics, algorithms, and software environments.

Performance Optimization of Problems in Computational Science And Engineering

- **Activities** (past, *on-going, +just started)
 - **Derive novel dynamic loop scheduling techniques*
 - Theoretical perspective, application and system integration
 - New algorithms are based on probabilistic analyses and are robust (high degree of generality, theoretical constraints of model are relaxed)
 - New algorithms are adaptive and effective in heterogeneous environments characterized by irregular and highly unpredictable behavior
 - Performance analysis, evaluation and prediction, from analytical and experimental perspective
 - **Optimization through the use of machine learning in the automatic selection of dynamic scheduling algorithms ==>> autonomic computing*
 - *Develop dynamic load balancing tools and libraries*
 - **For cluster applications in (C, Fortran, Matlab) + MPI*
 - For enhanced functionality of systems: Hector; DMCS/MOL; **Loci*
 - *Participants: faculty, researchers and graduate students at MSU (CCS, HPC2,...), other universities and government labs*

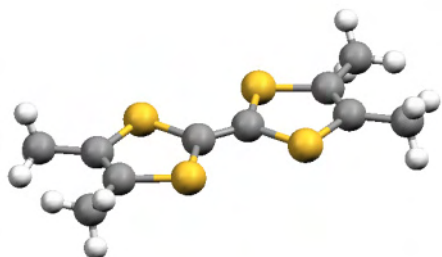
Performance Optimization of Problems in Computational Science And Engineering

Applications/Collaborations/Grants

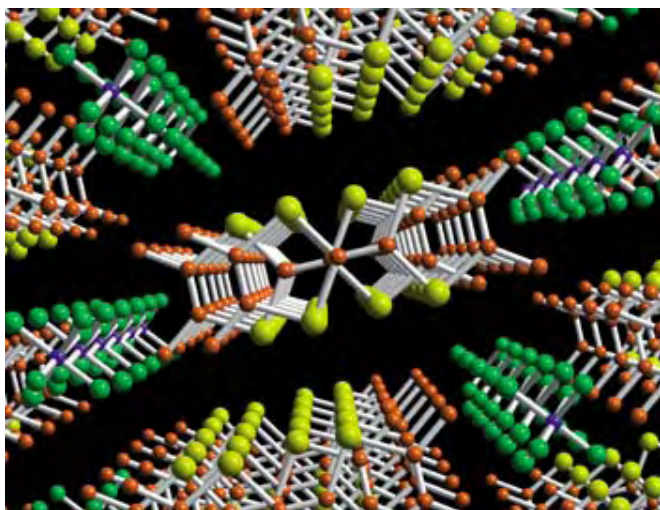
- *Applications*: N-body simulations; CFD simulations; Quantum physics *Astrophysics *Computational statistics *Image processing +Design optimization +Computational mathematics
 - Simulation of quantum trajectories for electron scattering problems, Analysis of Gamma ray burst profiles, Validation of statistical techniques for nonlinear vector time series, Simulation of PDE-techniques for image restoration, Design optimization of a parallel hybrid electric vehicle
- *Collaborations*: national (Cornell, College of William and Mary, ANL, ...), and international (U. Amsterdam, EPFL, U. Cork, T.U. Chemnitz, U. Bayreuth, ...)
- *Grants*: National Science Foundation (CAREER, ITR, and others)

Torsten Clay (Physics and Astronomy)

Clay group: molecular conductors, superconductors;
Quantum Monte Carlo, many-body electron methods



TMTSF molecule: typical building block for molecular SC's



Molecules combined into crystal. Strongly anisotropic in structure.

Recent Projects

1. RTC, RP Hardikar, *Phys. Rev. Lett.* **95**, 096401 (2005).

Electron-phonon (e-ph) interactions present in all molecular superconductors are usually expected to lead to insulating states. A challenge for the theory of superconductivity is *how to get a metallic state*.

We show that in one of the most basic models (Hubbard-Holstein model), the presence of *both* electron-electron (e-e) and e-ph interactions can give a novel metallic state adjacent to the Peierls and Mott insulating states.

2. RTC, S Mazumdar, *Phys. Rev. Lett.* **94**, 207206 (2005).

A new class of molecular “ladder” materials feature an unusually large spin gap (non-magnetic ground state). We explain this state occurs through *cooperation* of e-e and e-ph interactions. The gap forms due to singlet bonds between electrons along the ladder, which may be related to superconducting pairing in similar materials.

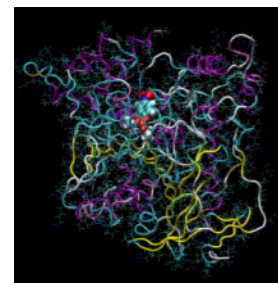
Supported by ACS (Petroleum Research Fund)

Steven R. Gwaltney

Department of Chemistry

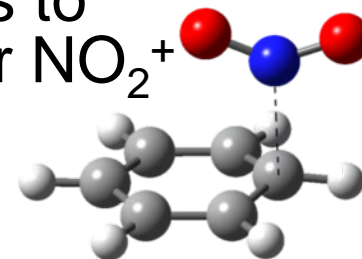
Modeling pesticide interactions with esterases

Using molecular dynamics simulations to determine how organophosphate insecticides bind to acetylcholinesterase



Mechanism of nitration reactions

Use electronic structure theory calculations to determine the potential energy surfaces for NO_2^+ reacting with substituted benzenes.



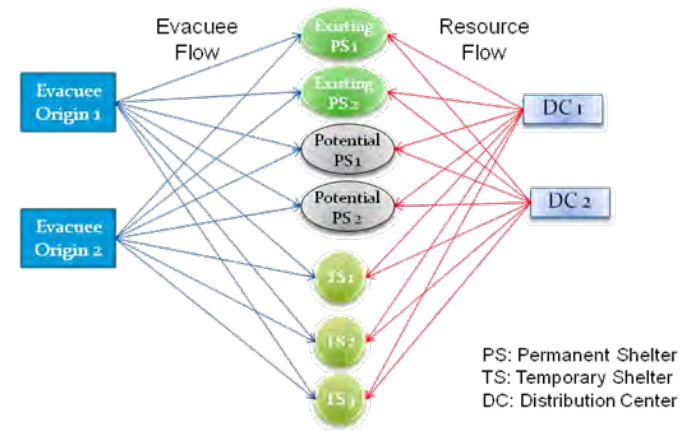
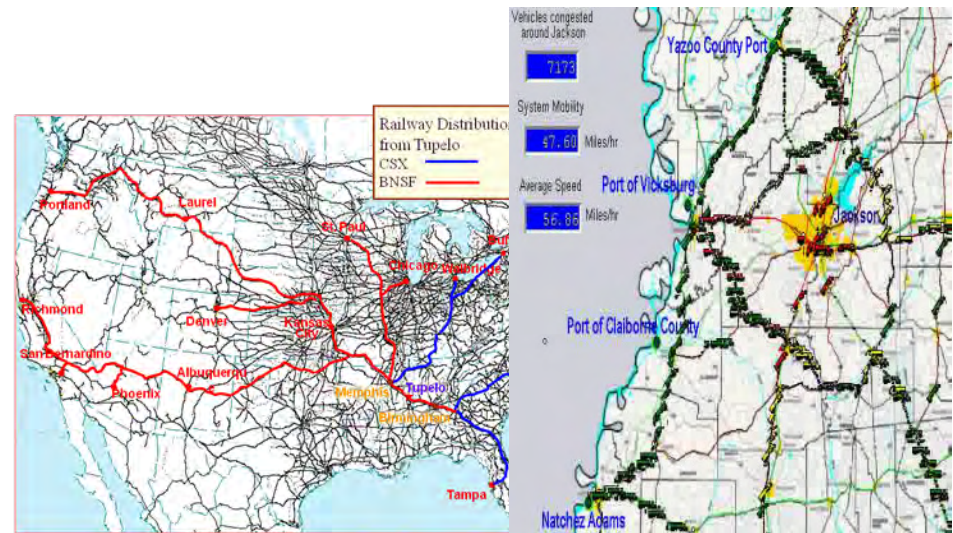
Excited state simulations

Calculate the spectra of dibenzoborole derivatives to determine the cause of their large blue shift in fluorescence upon complexation

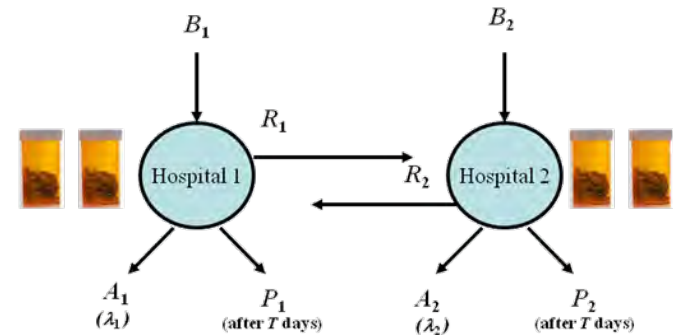


- **Optimization and Simulation for Transportation and Logistics Analysis**

- Automotive Distribution Network Design: A Perspective from Mississippi
- Alternate Route Planning Technology to Facilitate Highway Transportation of Cargo, Vehicles and Personnel during National Emergencies
- Sheltering Network Design and Management Responding to Natural Disasters



- Supply Chain Management through Optimization and Simulation
 - Lateral Transshipment for Slow-Moving Critical Medical Items
 - Geographic Information Systems Capability of Demonstrating the Current and Alternative Supply Chains for A Furniture Manufacturing Company
 - Algorithms for the Split Delivery Vehicle Routing Problem



$$P: \min Z^P = \sum_{g=0}^N \sum_{j=0}^N c_{gj} x_{gj} - \sum_{i=1}^N \pi_i \rho_i - \mu \quad (2.1)$$

$$\text{s. t. } \sum_{j=1}^N x_{0j} = 1, \sum_{j=1}^N x_{j0} = 1 \quad (2.2)$$

$$\sum_{j=1}^N x_{gj} = \sum_{j=1}^N x_{ji} = y_i \quad i = 1, \dots, N; \quad (2.3)$$

$$a_i \leq d_i y_i \quad i = 1, \dots, N; \quad (2.4)$$

$$\sum_{i=1}^N d_i - (K-1)Q \leq \sum_{i=1}^N a_i \leq Q; \quad (2.5)$$

$$u_i - u_j + (N+1)x_{ij} \leq N \quad i, j = 1, \dots, N; \quad (2.6)$$

$$x_{gj}, y_i \in \{0,1\}; a_i, u_i \geq 0 \quad i, j = 1, \dots, N.$$

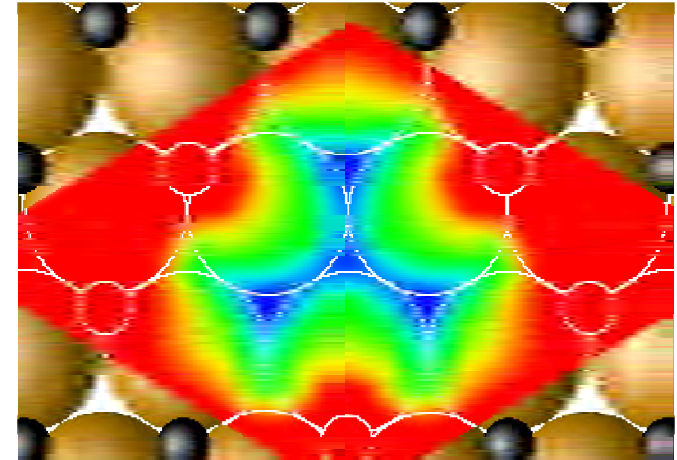
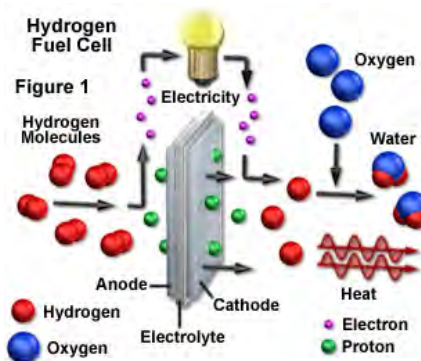
Seong-Gon Kim (Physics and Astronomy)

Students: Jeff Houze, Bohumir Jelinek, Amber Benson, Amitava Moitra

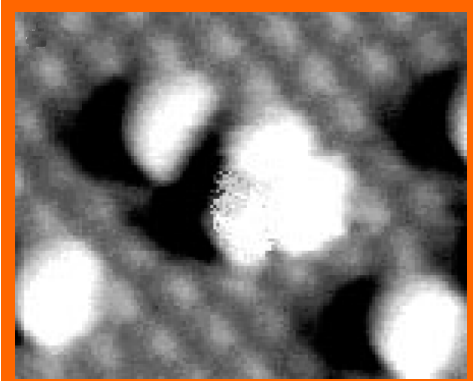
Postdoc: Sungho Kim

Quantum simulation of Hydrogen Catalysis

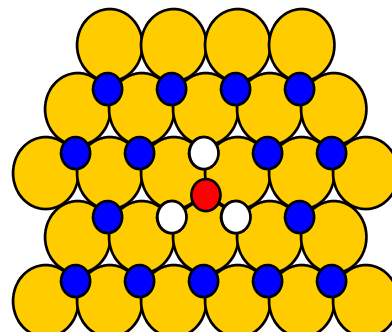
Objective: *To perform quantum mechanical simulations to better understand the hydrogen catalysis on metal surfaces*



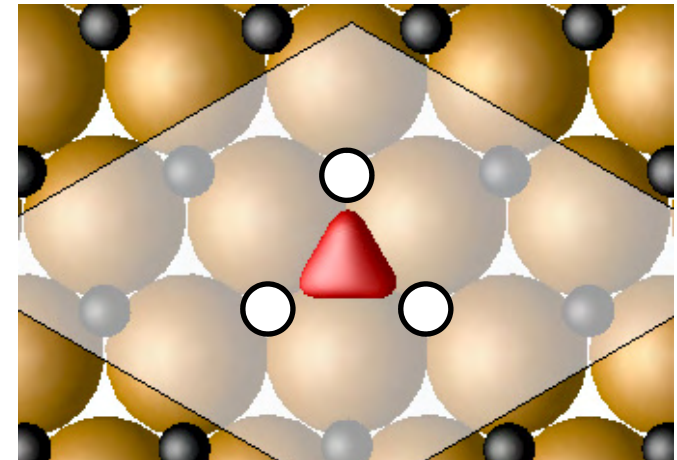
Potential energy for a single H atom in three empty sites



STM image of divacancy (2V) on Pd(111) surface



Quantum model of 2V = one H in three empty sites

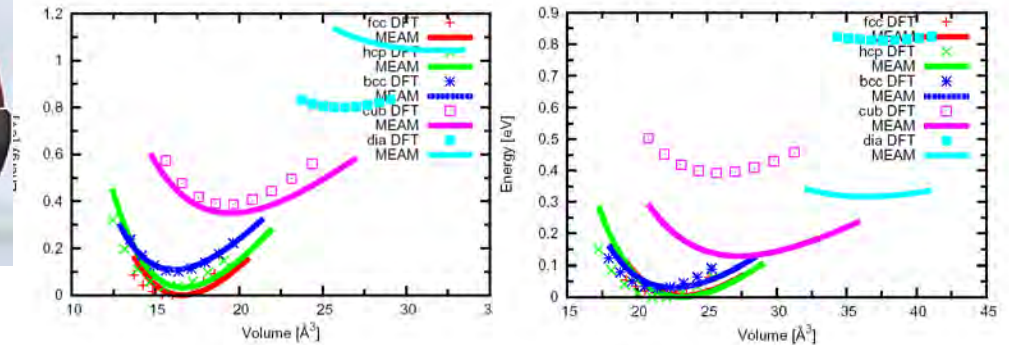


Ground state of H atom of divacancy showing three exposed fcc sites

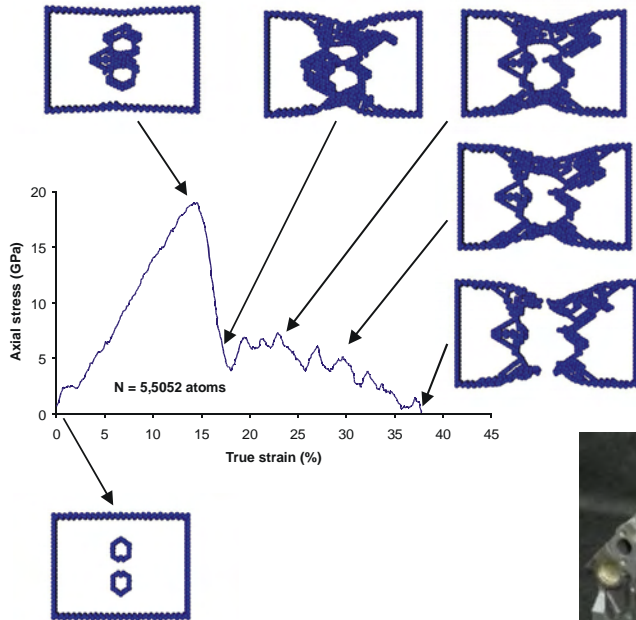
Seong-Gon Kim (slide 2)

Light-weight High-strength Steel and Mg Alloys for Automotive Applications

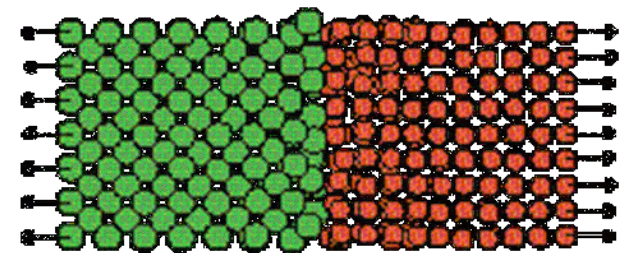
Objective: To employ quantum mechanical material modeling to reduce the weight of components



Validation of Modified Embedded Atom Method (MEAM) potential for Al and Mg against First-principles method



Atomistic simulation of crack propagation under tensile stress

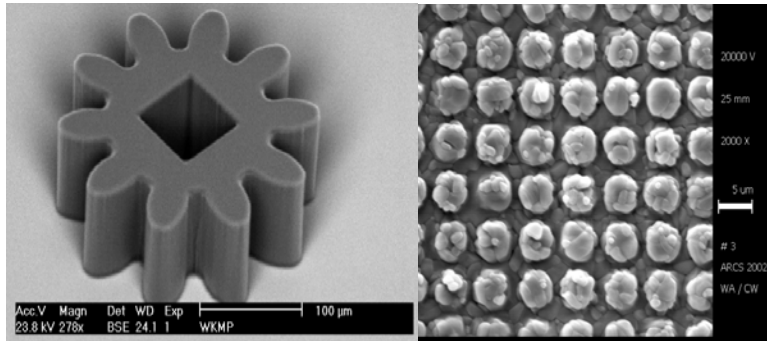


Atomistic simulation of interfacial debonding and fracture

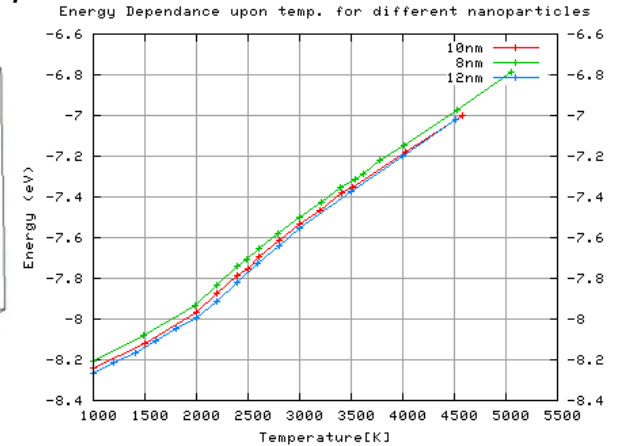
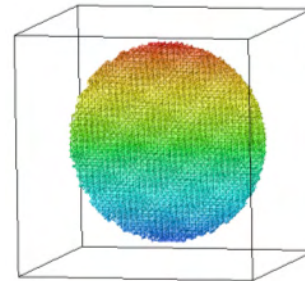
Seong-Gon Kim (slide 3)

Atomistic Simulation of Nanopowder Sintering

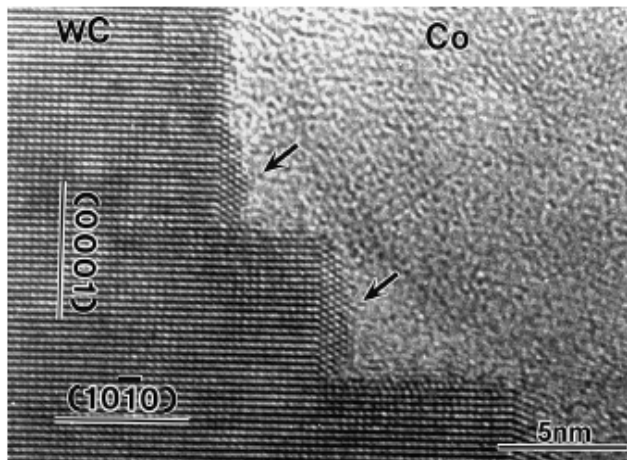
Objective: *To perform realistic atomistic and quantum mechanical simulations to better understand the fundamental mechanisms and optimize nanopowder sintering process*



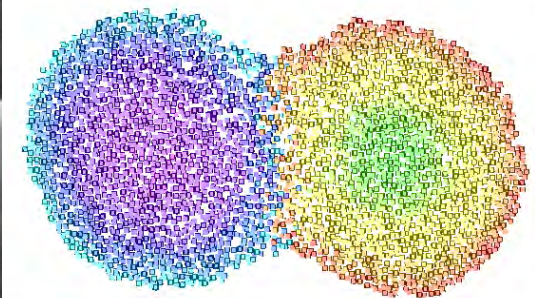
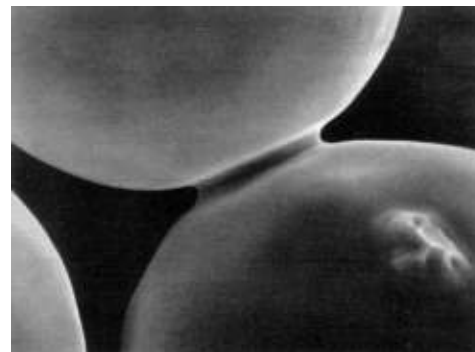
Metal parts manufactured from powder sintering process



Melting of a single tungsten 10 nm nanoparticle



TEM image of vanadium atoms acting as the inhibitor of grain growth of WC/Co system

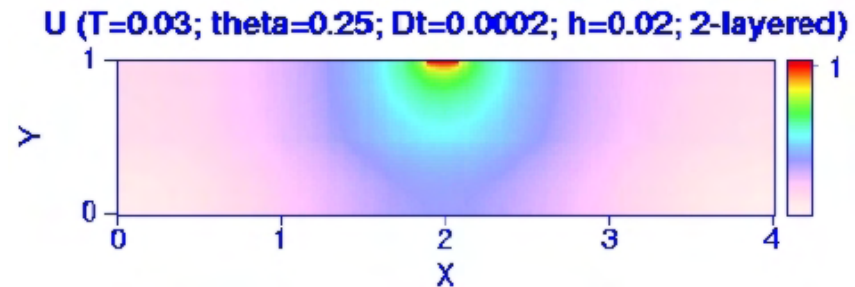
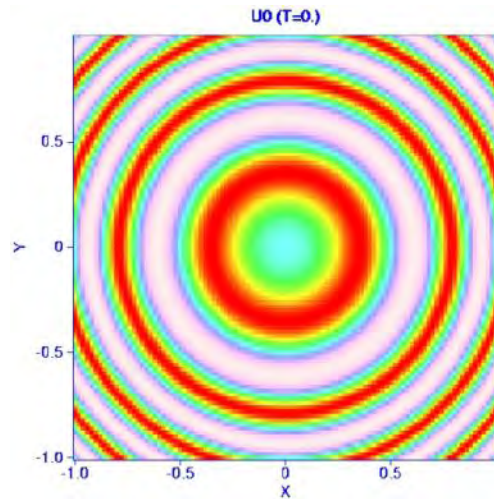


Sintering of two nickel microparticles (experiment) and two tungsten nanoparticles (simulation)

Hyeona Lim

- **Propagation on Viscous and and Nonviscous Waves**

Develop efficient high-order numerical methods and associated algorithms for viscous (microscale heat transfer) waves and nonviscous (acoustic waves) wave equations.



Simulation of Acoustic waves (left) and microscale heat transfer for double layered material (right)

Hyeona Lim (2)

- **Image denoising and segmentation**

Develop efficient partial differential equation based models and their algorithms for image denoising and image segmentation.

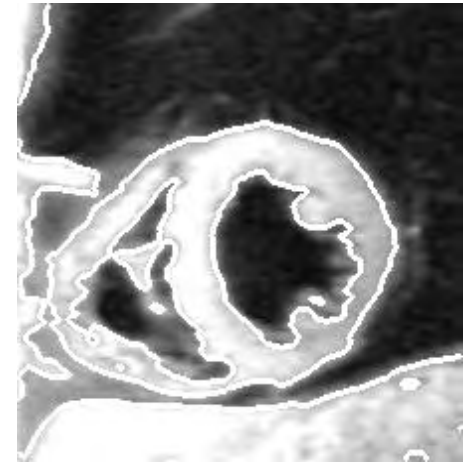
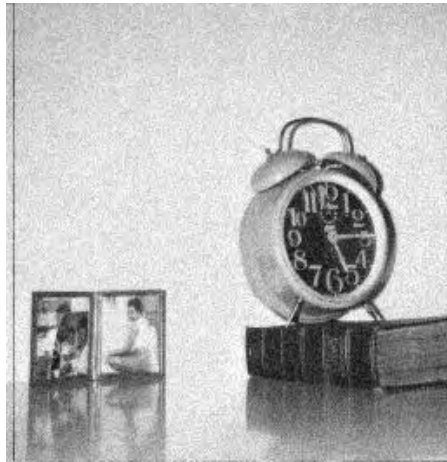
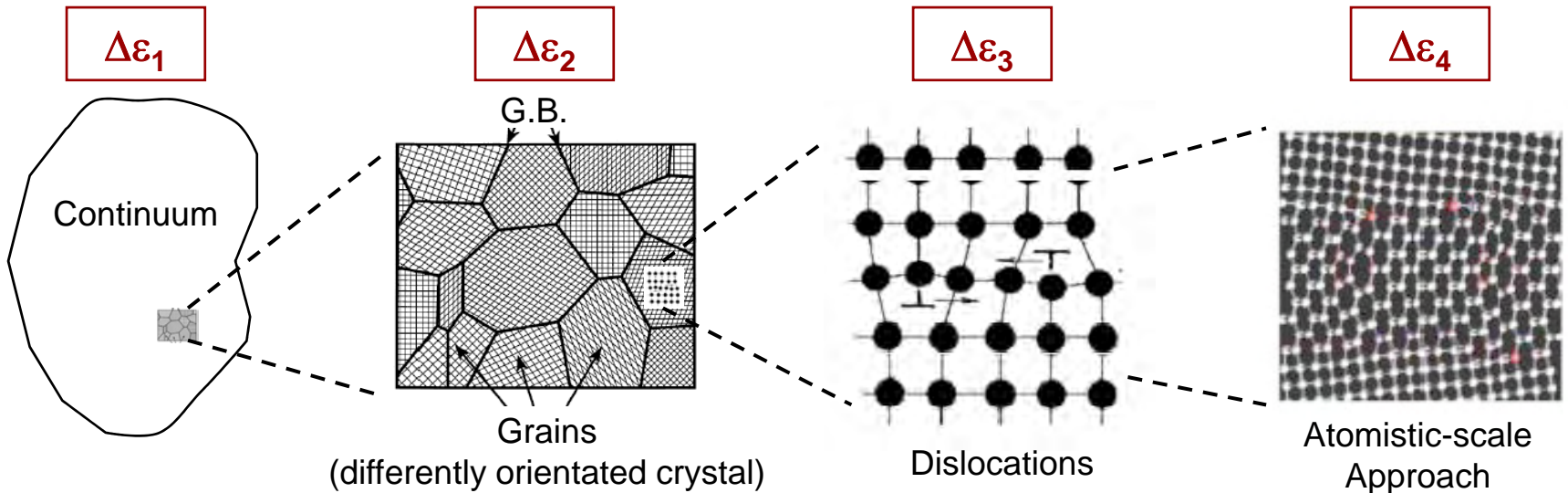


Image denoising (enhancement) for clock image (left-noisy, middle-enhanced) and cardiac image segmentation (right)

Hyeona Lim (3)

- Error Analysis on Multiscale Modeling**

Develop mathematical analysis of the error $\Delta\varepsilon$ introduced by the different models and computational methodologies at different scales of deformation and damage process for better design optimization of lightweight vehicles.



- Trend Study in a Periodic Time Series Regression Model

$$X_{mT+v} = \mu_v + \alpha_v(mT + v) + \delta_{mT+v} + \varepsilon_{mT+v}$$

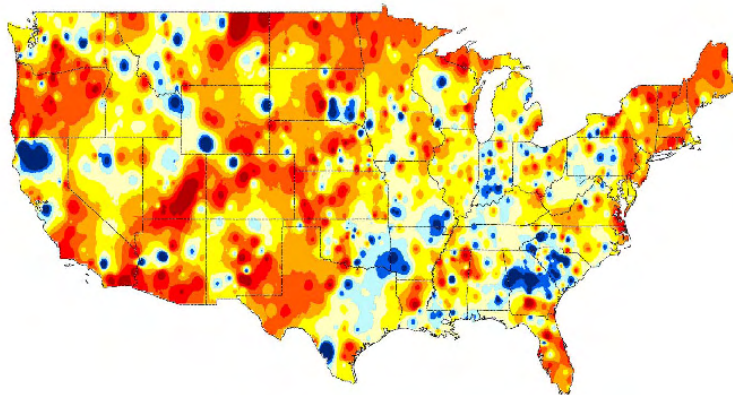


Figure 3: Raw Annual Trends

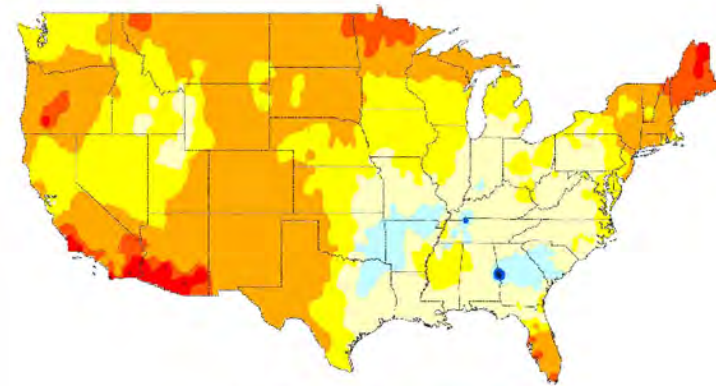
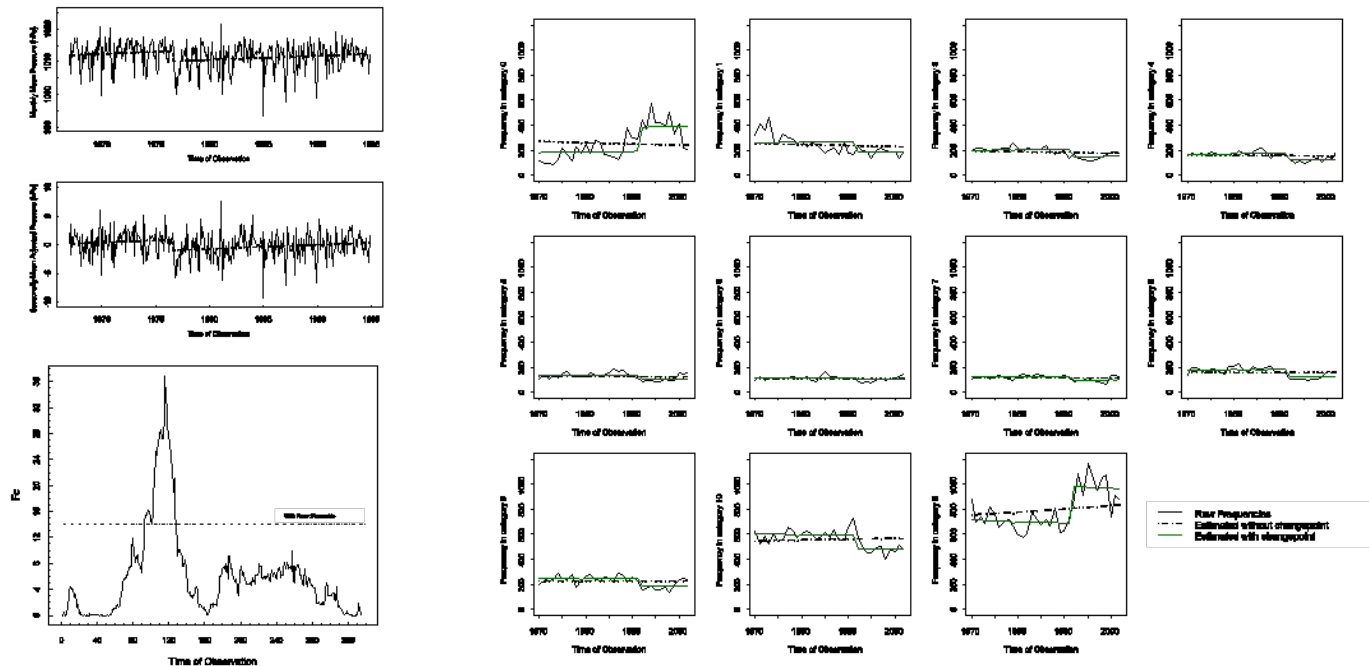


Figure 4: Smoothed Annual Trends

Annual temperature trend estimates in USA (left) and its spatially smoothed trend estimates (right)

• Changepoint Detection of Climate Time Series

- A changepoint is a time at which the structural pattern of a time series changes. It can be induced from station moves, instrumentation/observer changes, and changes in observation practices.
- **Develop statistical tests for undocumented changepoints for climatic time series.**



Changepoint detection for a monthly mean atmospheric pressure series (left) and a yearly frequency of cloudiness conditions (right)

TR: “Non-Equilibrium Surface Growth and the Scalability of Parallel Discrete-Event Simulations for Large Asynchronous Systems”, DMR Award#0426488
Gyorgy Korniss (Rensselaer Polytechnic Institute), **Mark Novotny** (Mississippi State University)
ark

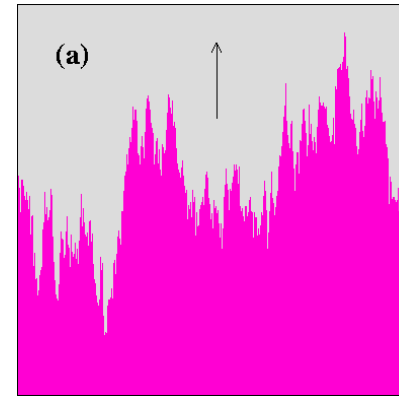
Parallel discrete-event simulation is an invaluable general tool to investigate the dynamic behavior of complex systems. Such systems include battle-field models, models for the spread of diseases and epidemics, cell-phone communication networks, dynamics of materials, and financial markets - some of these being dauntingly relevant in our everyday life.

As tomorrow’s state-of-the-art massively parallel architectures will have about a million CPUs (e.g., IBM’s Blue Gene Project), the design of scalable algorithms becomes an extremely challenging task. In particular, synchronizing that number of CPUs using some kind of central control is beyond hope.

We constructed a novel synchronization protocol in which CPUs operate *autonomously* without any centralized control. We achieved this by requiring each CPU to communicate only with a few others through a “*small-world*” network. This type of complex network (producing the “six degrees of separation”) is well known from social systems to be capable of facilitating the spread of information in a highly efficient manner. Providing a near-uniform progress of the CPUs, this method is scalable in both the simulation and the data collection phases of the algorithm.



regular one-dimensional communication topology



“small-world” topology when random links are added

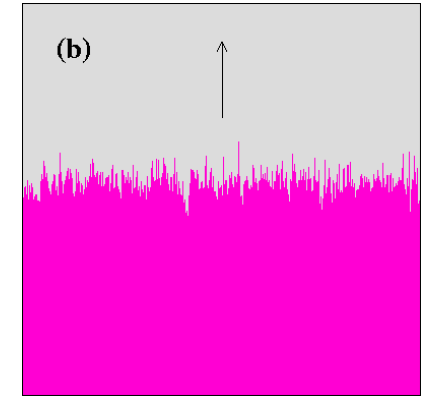


Figure 1 [Horizontal axis: individual CPUs; vertical axis: progress of the simulation of the individual CPUs.] **(a)** When compute nodes only communicate with local neighbors, the spread of the progress of the simulation increases with the number of nodes, making continuous data retrieval not scalable. This corresponds to a wildly fluctuating simulated time horizon (large spread of the progress of the individual CPUs). **(b)** When each node is also required to communicate with a randomly chosen one (resembling a “*small-world*” network), *synchronization emerges spontaneously*, without a central command.

ABSL/CERDEC contract

Novotny and Wu

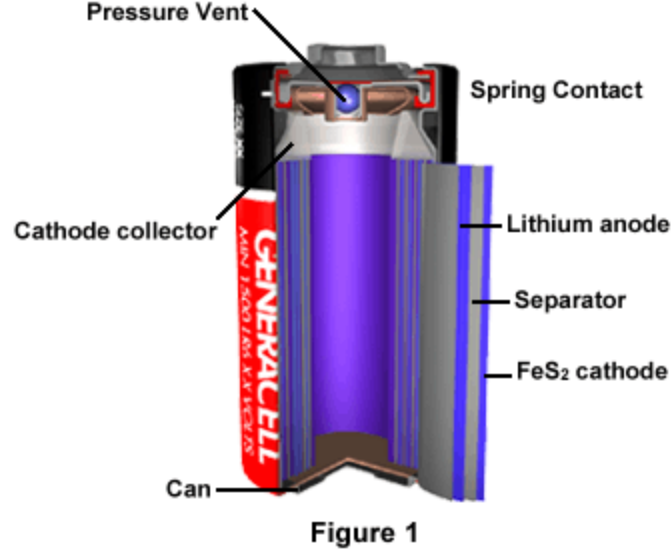
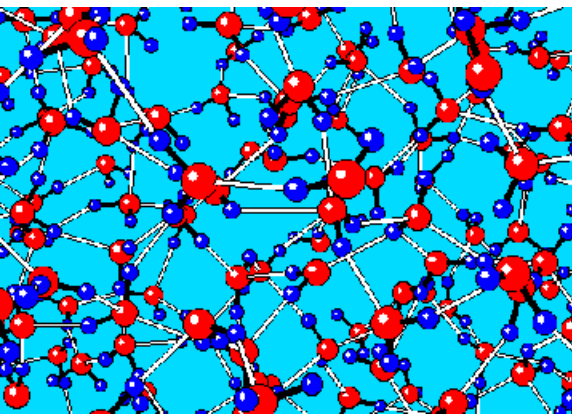
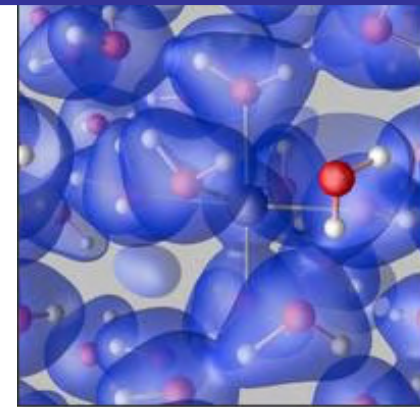
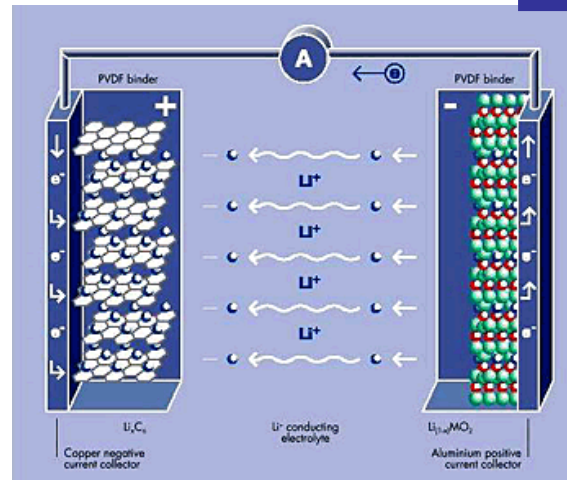
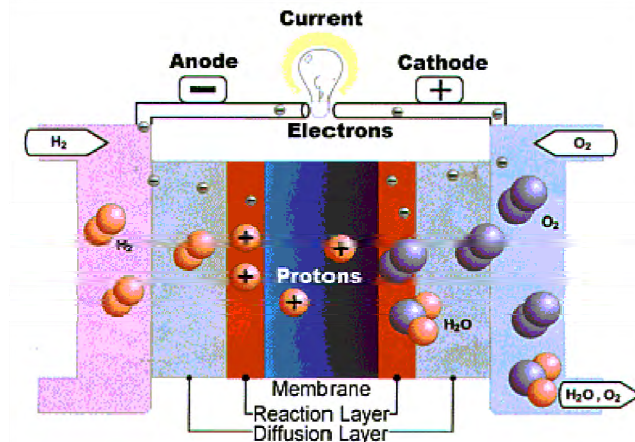


Figure 1



Monies starting in July 2006



- Calculations for lithium ion batteries (molecular dynamics and dynamic Monte Carlo atomistic simulations)
- Calculations of fuel cell/battery combinations (device scale simulations)

Physical Small-World-like Network Research with High-School Students

DMR-0426488 (ITR) [Gyorgy Korniss](#) ([Rensselaer](#)), [Mark Novotny](#) ([Mississippi State University](#))

JOURNAL OF APPLIED PHYSICS 97, 10B309 (2005)

Magnetic small world nanomaterials: Physical small-world networks

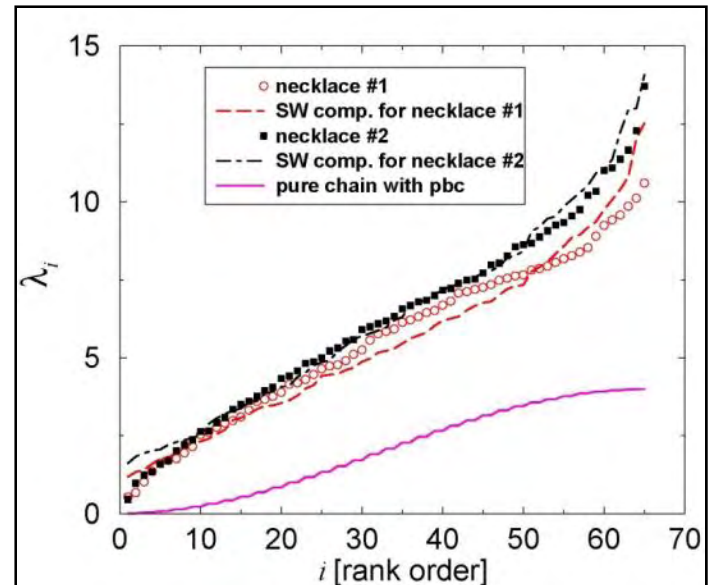
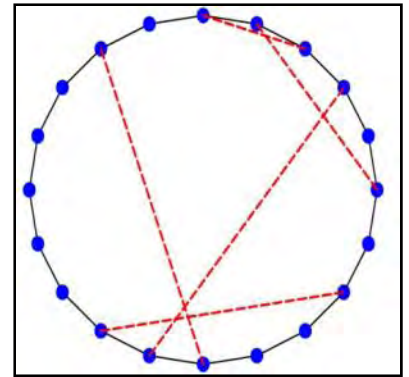
M. A. Novotny,^{a)} X. Zhang, J. Yancey, T. Dubreus, **M. L. Cook, S. G. Gill, I. T. Norwood,**
and **A. M. Novotny**

Department of Physics and Astronomy, ERC Center for Computational Sciences, Mississippi State University, Mississippi State, Mississippi 39762-5167

G. Korniss^{b)}

Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, New York 12180-3590

(Presented on 10 November 2004; published online 4 May 2005)



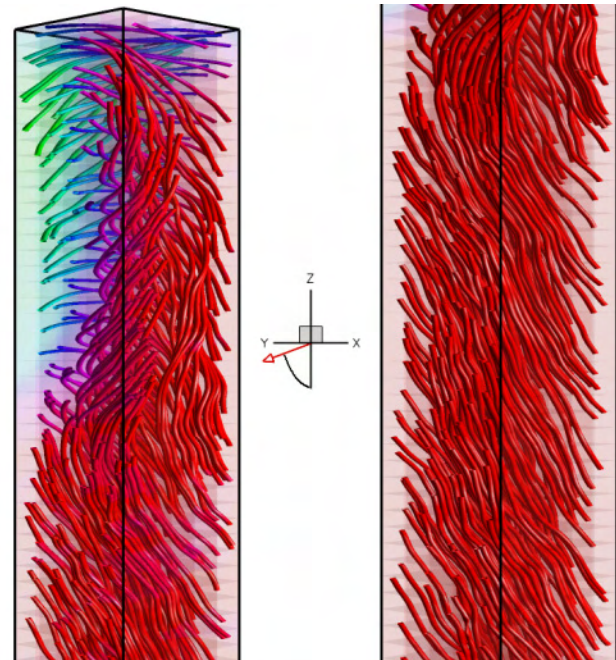
Four high-school students at Mississippi State, pictured with one of their created physical small-world networks, worked with the PIs for one summer. Their work, shown in the figure, for the eigenvalue spectrum λ_i of the SW-network Laplacian, was published in *J. Applied Physics* in 2005, shown with their names highlighted.

Visualization of Magnetization Switching in a Misaligned Iron Nanopillar

Mark A. Novotny, Mississippi State University

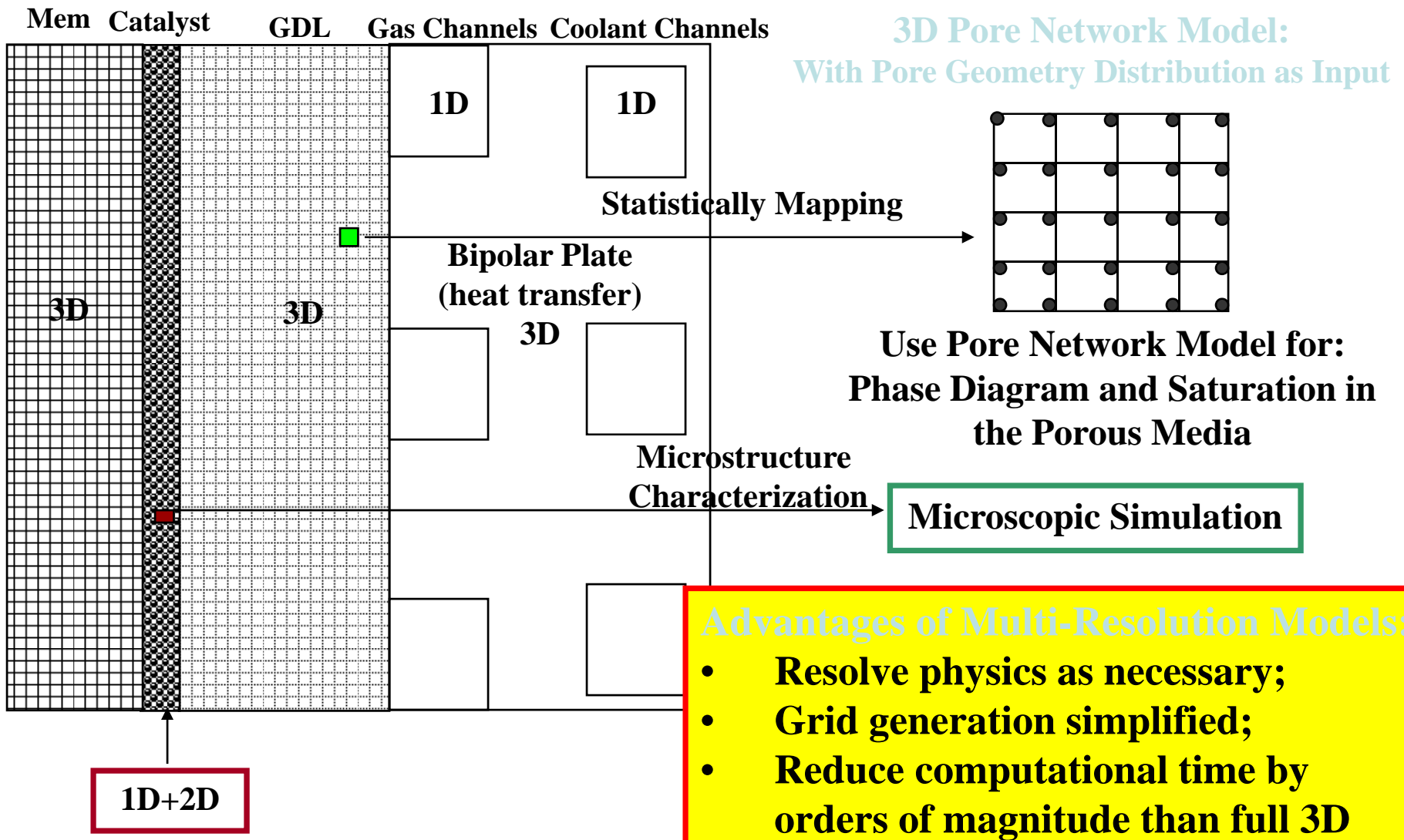
Per Arne Rikvold, Florida State University, DMR-0120310

Magnetic nanoparticles are promising materials for ultra-high density magnetic recording media and magnetic RAM. Here we show a visualization of the internal magnetic flux lines in a simulated 9 nm x 9 nm x 150 nm Fe nanopillar, modeled on particles produced experimentally at Florida State University. The simulations use a stochastic differential equation (Landau-Lifshitz-Gilbert equation) for the local magnetization, which includes exchange and magnetostatic interactions, anisotropy, and random thermal fluctuations.

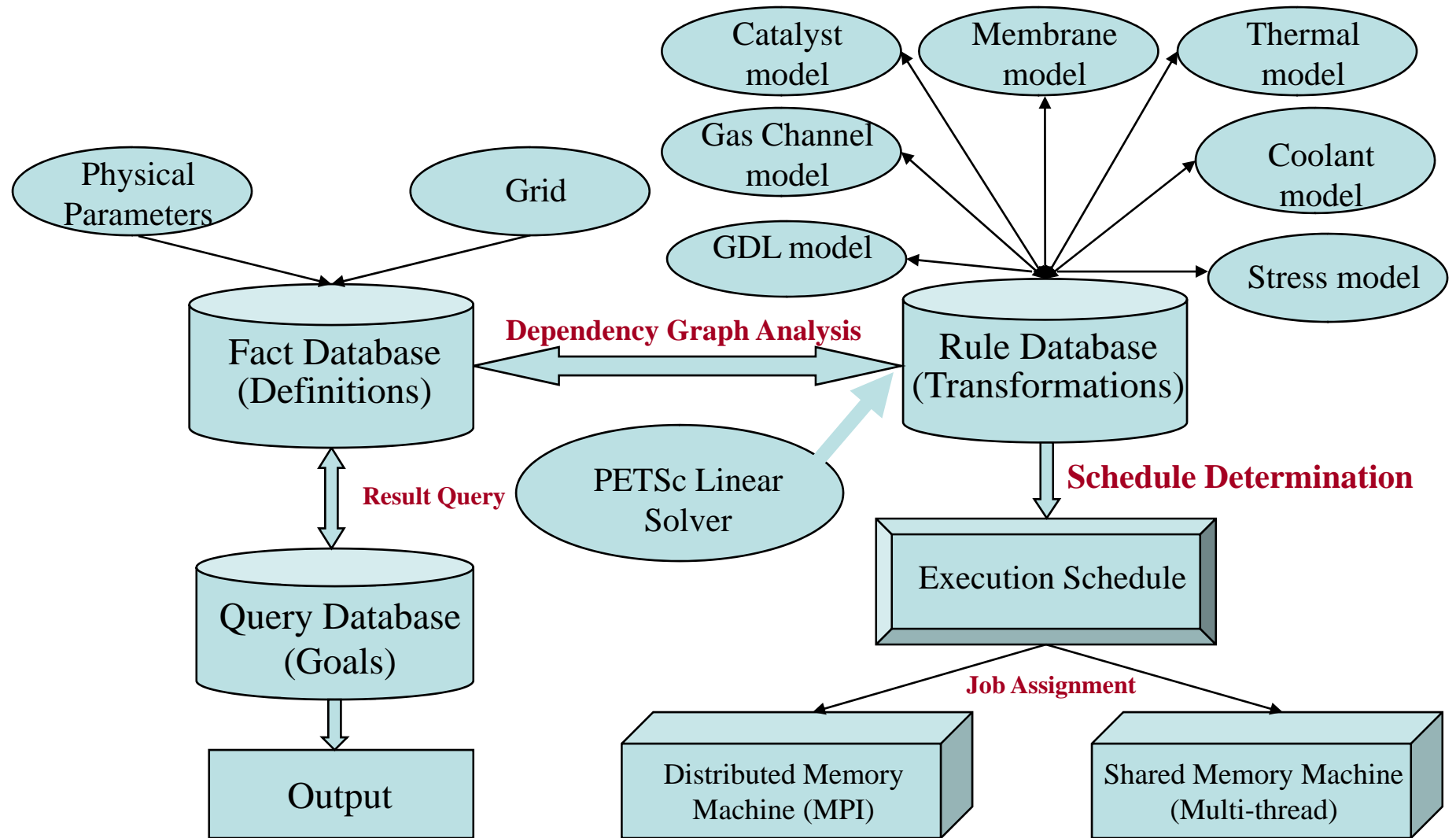


Magnetic flux lines in an Fe nanopillar in an applied magnetic field that makes 75° with the long axis (red arrow in the middle). The pillar is in the metastable state, with most of its spins aligned antiparallel to the z-component of the applied field. Green: stable direction. Red: metastable direction. Left: top of pillar. Right: middle of pillar.

Multi-Resolution Fuel Cell Model



Loci Based Fuel Cell Simulation



Simulation Aided Optimal Design

Parameters and Variables to Be Optimized:

Operating Conditions: Inlet gas composition, temp., flow rate;
Coolant type, coolant inlet temp., flow rate;
Water residual content affected by shutdown

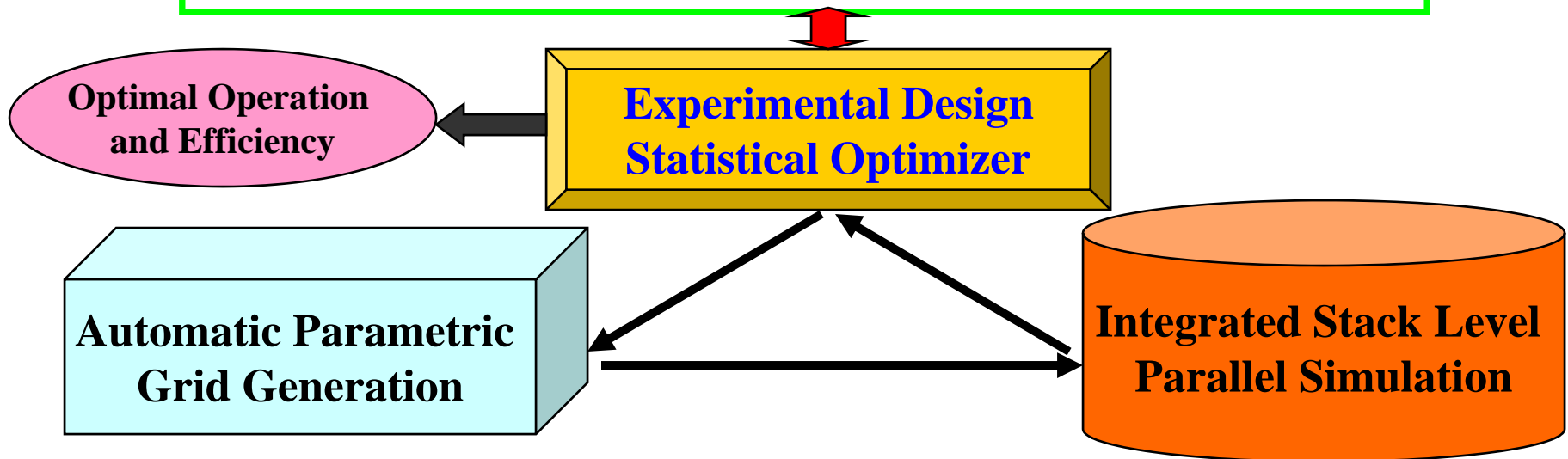
Gas Channels: Channel patterns, channel width and height

Coolant Channels: Channel patterns, channel width and height

GDL: Thickness, pore size dist., hydro-phobic/phobic pore ratios

Catalyst: Platinum and carbon particle sizes, platinum loading

Membrane: Thickness



Reaction Diffusion Equations --- Steady States

Ratnasingham Shivaji

Objectives: To analyze the structure of positive solutions to classes of steady state reaction diffusion models arising in population dynamics and nonlinear heat generation

• Population Dynamics



• Nonlinear Heat Generation

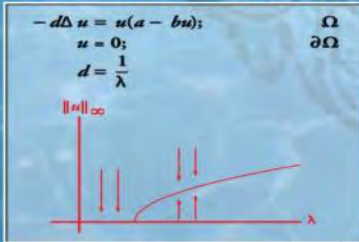


Population Dynamics

Objectives: To analyze the structure of positive solutions to classes of steady state reaction diffusion models arising in **population dynamics**.

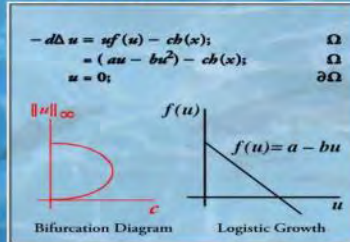
Population Dynamics

Bifurcation Diagram: Logistic Growth

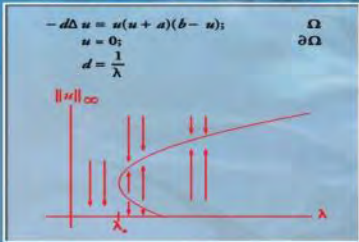


Harvesting

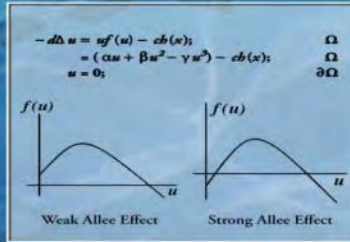
Logistic Growth



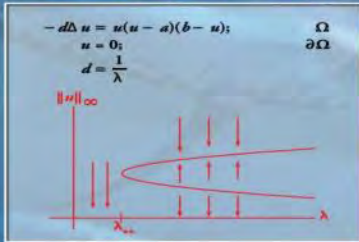
Bifurcation Diagram: Weak Allee Effect



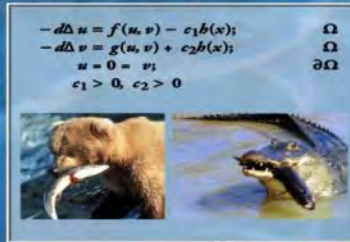
Allee Effect



Bifurcation Diagram: Strong Allee Effect



Predator Prey Systems



'No place for fish to hide'

Damage to large species might be permanent

By Dan Vergaman USA TODAY THURSDAY, MAY 15, 2003 11D



Commercial fishing has wiped out 90% of the world's populations of large fish, scientists say. Popular species in danger include tuna, cod, swordfish, marlin, halibut, skate, flounder and shark. The report, published today in the journal *Nature*, suggests that international efforts to manage coastal and deep-ocean fisheries have not kept up with advances in commercial fishing and over-sized fishing fleets. The study analyzed 13 fisheries, sea regions that are home to large-scale fishing operations.

Most surprising to the researchers is the finding that industrialized fishing essentially has spread to every coastal and ocean source in the world. Further, industrial fishing appears to deplete fish communities within only 10 to 15 years' time.

"There's no place left in the world for fish to hide," says lead author and fisheries biologist Ransom Myers of Canada's Dalhousie University.

Popular species on decline in 13 fisheries analyzed

- Atlantic cod
- Barndoor skate
- Skipjack tuna
- Broadbill swordfish
- Bluefin tuna
- Yellowfin tuna

The study, conducted over 10 years, used industry data from over five decades to look at fisheries from the North Atlantic to the Antarctic Ocean.

Myers warns that at present rates of fishing, some species will disappear from supermarket shelves and that some sharks, like the hammerhead, may become extinct. He says excessive fishing arises from:

- Advances in fishing technology such as sonar and advanced longline and deep-sea trawling techniques.
- Too many ships in fishing fleets.
- The failure of nations to agree to manage fish populations.

Industry spokeswoman Linda Candler of the National Fisheries Institute calls the study results "overstated" and says they don't square with industry estimates of fish-population recovery in some locales. The study is out of context and doesn't recognize the reality that fisheries are now part of the commercial fishing industry.

However, fisheries biologist Andrew Rosenberg of the University of New Hampshire, who was not involved in the study, says the study suggests that excessive fishing already may have reduced some fisheries to unrecoverable levels. Even though fish may reproduce in greater numbers to replace yearly losses — a point also raised by Candler — fish don't magically replace themselves completely every year, Rosenberg says. Depleting them until it is clear the population is in peril may ruin a fishing region forever, he says.

"It's not a story of fishermen doing anything wrong," Rosenberg says. "They need to pay their mortgages too, but there are simply too many boats chasing too few fish."

Nationwide, the \$29 billion seafood industry employs about 250,000 people. Medical researchers have found health benefits from eating fish, which has driven U.S. consumption.

Worldwide, fish is a diet staple. About 78 million tons was caught in 2000, not including China's reported catch of 17 million tons, a number widely regarded as an overestimate. Conservationists warn that these numbers represent a decline to fishing levels of a decade ago, perhaps a sign that more international agreement to manage fisheries are needed, in fisheries management and conservation areas. Such efforts have

References

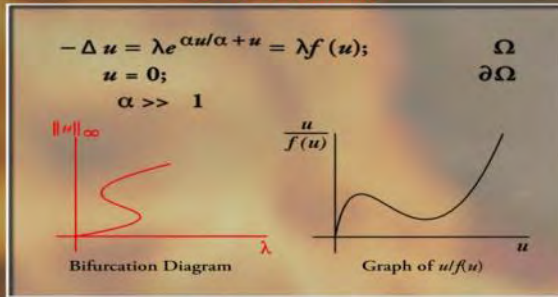
- [1] Diffusive logistic equation with constant yield harvesting, J. Steady States, S. Orizantzi, J. Shi and R. Shivaji, Trans. Amer. Math. Soc. 354, (2002), pp. 3601-3619.
- [2] Population Models with Diffusion and Constant Yield Harvesting, A. Collins, M. Gilliland, C. Henderson, S. Krone, J. McFerrin and K. Wampler, Rose-Hulman Institute of Technology Undergraduate Math Journal, Vol.5, Issue 2, 2004.
- [3] Positive Solutions to a Diffusive Logistic Equation with Constant Yield Harvesting, T. Ladner, A. Little, K. Marks and A. Russell, Rose-Hulman Institute of Technology Undergraduate Math Journal, Vol.6, Issue 1, 2005.
- [4] Population Dynamics with Nonlinear Diffusion, D. Perry, J. Schaefer, B. Schilling, and M. Williams, Rose-Hulman Institute of Technology Undergraduate Math Journal, Vol.7, Issue 2, 2006.
- [5] Persistence in reaction diffusion models with weak Allee effect, J. Shi and R. Shivaji, J. Math. Biol. 52 (2006), 807-829.
- [6] Population Models with Diffusion, Strong Allee Effect and Constant Yield Harvesting, Jaffar Ali, R. Shivaji and Kellan Wampler, submitted.
- [7] Diffusive logistic equation with discontinuous constant yield harvesting, Jaffar Ali, David Perry, Sarah Sasi, Jessica Schaefer, Brian Schilling, R. Shivaji and Matthew Williams, in preparation.



Nonlinear Heat Generation

Objective: To analyze the structure of positive solutions to classes of steady state reaction diffusion models arising in nonlinear heat generation.

Combustion



Nonlinear Diffusion

Combined effects of Φ and f

$$-\nabla \cdot (d\phi(u)\nabla u) = f(u); \quad \Omega$$

$$u = 0; \quad \partial\Omega$$

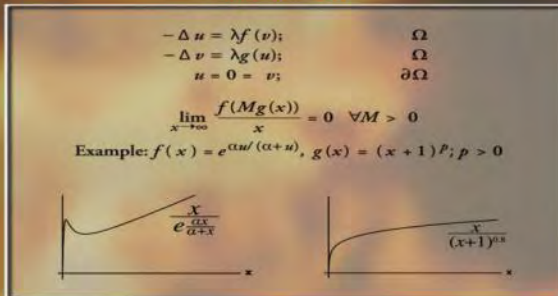
Uniqueness for $\lambda \gg 1$

$$-\nabla \cdot (|\nabla u|^{p-2}\nabla u) = \lambda f(u); \quad \Omega$$

$$u = 0; \quad \partial\Omega$$

$$\left(\frac{x^{p-1}}{f(x)}\right)' > 0; \quad x \gg 1$$

Combined Nonlinear Effects Multiplicity



Systems-Existence and Multiplicity

$$-\nabla \cdot (|\nabla u|^{p-2}\nabla u) = \lambda_1 f(v) + \mu_1 h(u); \quad \Omega$$

$$-\nabla \cdot (|\nabla v|^{q-2}\nabla v) = \lambda_2 g(u) + \mu_2 \gamma(v); \quad \Omega$$

$$u = 0 = v; \quad \partial\Omega$$

$$\lim_{x \rightarrow \infty} \frac{f(M[g(x)]^{1/q-1})}{x^{p-1}} = 0 \quad \forall M > 0$$

Non-existence for $\lambda, \gg 1$

$$-\nabla \cdot (|\nabla u|^{p-2}\nabla u) = \lambda f(u, v); \quad \Omega$$

$$-\nabla \cdot (|\nabla v|^{q-2}\nabla v) = \lambda g(u, v); \quad \Omega$$

$$u = 0 = v; \quad \partial\Omega$$

$$f(u, v) \geq K_1 u^{p-1} - M_1$$

$$g(u, v) \geq K_2 v^{q-1} - M_2 \quad \forall u, v > 0$$

References

- [1] Brown K.J., Ibrahim M.M.A., and Shivaji R. S-Shaped bifurcation curves. *Nonlinear Anal. TMA*, Vol.5, No.5 (1981), 475-486.
- [2] Ramaswamy M., and Shivaji R. Multiple positive solutions for a classes of p-Laplacian equations. *Diff. and Int. Eqns.* 17 (2004), 1255-1261.
- [3] Jaffar Ali, Mythily Ramaswamy and R. Shivaji. Multiple positive solutions for classes of elliptic systems with combined nonlinear effects. *Diff. and Int. Eqns.* 19 (6) (2006), 669-680.

Lisa Wallace – Department of Biological Sciences

I. Evolutionary Diversification of *Schiedea* on the Hawaiian Islands

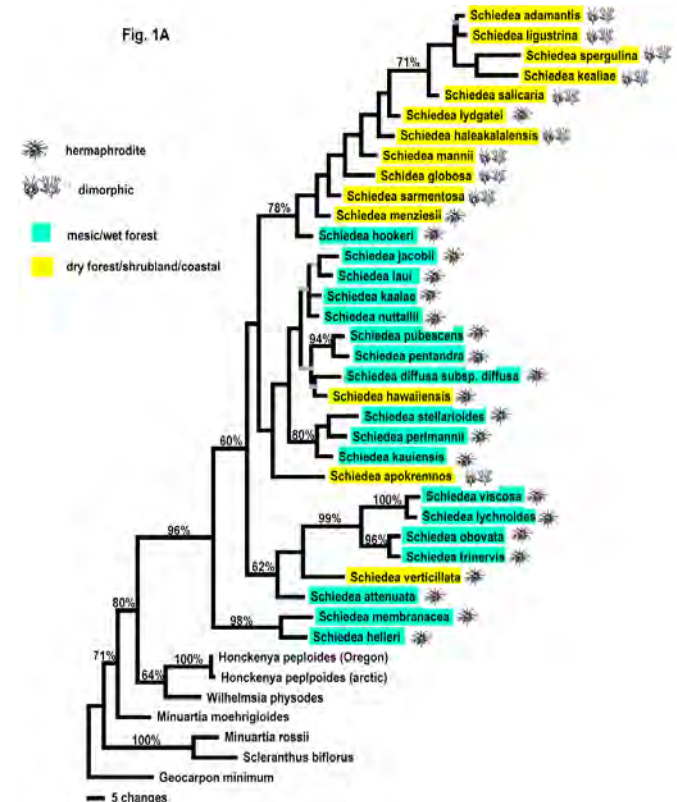
(Collabs. Drs. Molly Nepokroeff, Ann Sakai, Warren Wagner, & Steve Weller)



Photo: Warren Wagner

Schiedea, an endemic genus of the Hawaiian Islands, is a model system for understanding the mechanisms of plant evolution in island systems. We are interested in understanding how *Schiedea* evolved on the Hawaiian Islands and the reasons for the incredible diversity in breeding system and habitat exhibited by its members.

To address these questions, we are constructing an updated phylogeny based on a multi-gene dataset to test hypotheses about the correlated evolution of morphological characters and biogeographic patterns, and examining sequence variation at the intraspecific level to elucidate phylogeographic patterns within widespread species and dynamics of natural hybridization. We are also applying our understanding of genetic structure to the conservation of *Schiedea* through the use of spatially explicit techniques borrowed from the field of landscape ecology.



II. Conservation Genetics and Evolution of the California Channel Islands Flora

(Collabs. Drs. Kaius Helenurm and Mitchell McGlaughlin)

The California Channel Islands (map at right) are a unique archipelago because they exhibit a surprisingly high number of endemic plant species (15% of the flora) despite being very close to mainland California.

Research in this system is focused in two areas: 1) documenting population genetic structure and the impact of historical disturbances on the maintenance of genetic variation in rare species, and 2) addressing fundamental biogeographic questions of how and when endemic species evolve across the islands using *Lotus* species as model taxa and testing hypotheses of gene flow, genetic drift, and divergence.



Future diversity in *C. californicum*

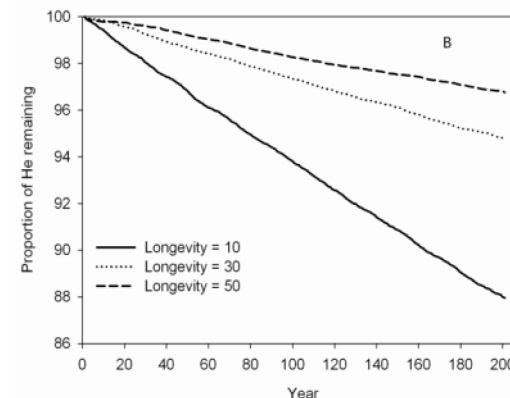
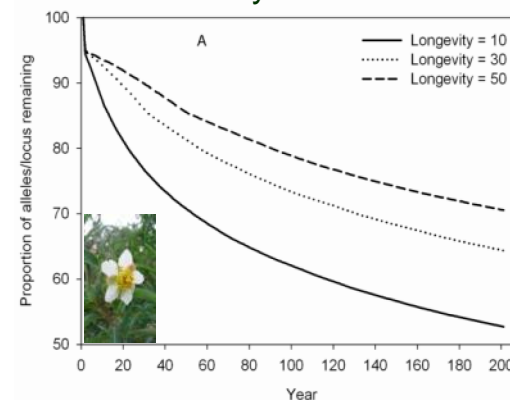


Table 1. Features of the California Channel Islands. Endemism is expressed relative to total native taxa.

Island	Age (my)	Distance (km)		Area (km ²)	Endemism (%)
		Nearest island	Mainland		
San Miguel	1.7	5	42	37	9.1
Santa Rosa	4.2	5	44	217	10.9
Santa Cruz	5.0	7	30	249	9.4
Anacapa	1.9	7	20	3	11.6
Santa Barbara	1.0 - 1.5	39	61	3	15.9
San Nicolas	0.6	45	98	58	13.0
Santa Catalina	3.2- 5.0	34	32	194	8.8
San Clemente	4.4	34	79	145	17.3



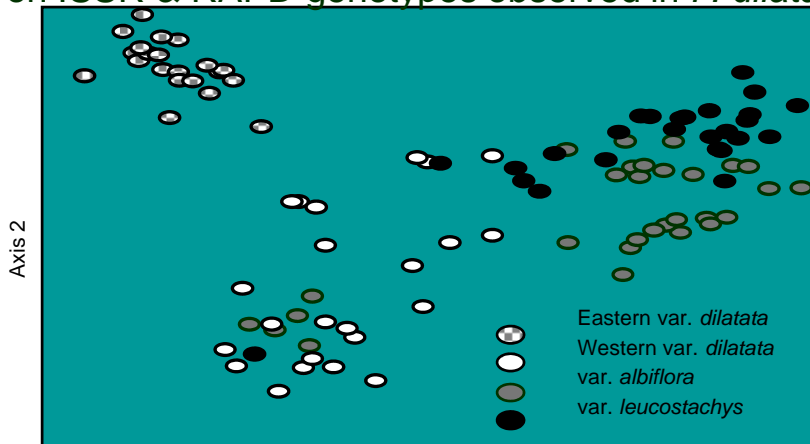
Lotus sp.

III. Speciation and Population Biology of *Platanthera* Orchids

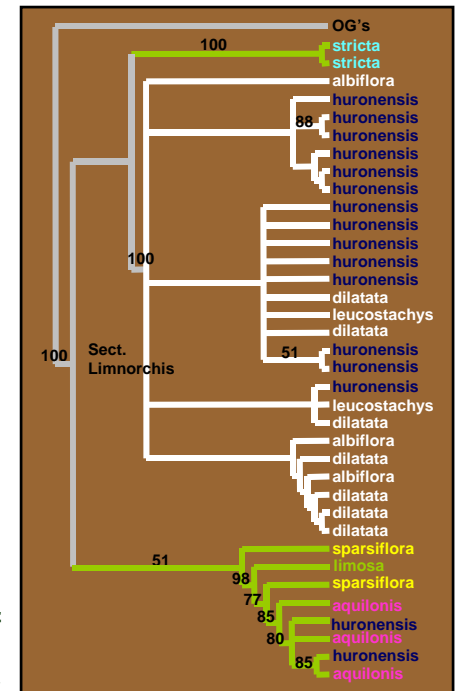


The Orchid family is among the largest and most diverse groups of flowering plants. My work, focused on section *Limnorchis* of the genus *Platanthera*, is directed at 1) resolving taxonomic confusion among *Platanthera* species through systematic studies of morphological and molecular data, 2) understanding genetic and ecological consequences of polyploidization in *P. huronensis* by characterizing morphological, ecological, and molecular genetic variation throughout the species' range and testing for phylogeographic patterns among independently derived lineages, and 3) studying how genetic drift and pollinator-mediated selection act to drive diversification in *P. dilatata*.

Plot of individuals from a multivariate PCoA based on ISSR & RAPD genotypes observed in *P. dilatata*



Axis 1



Strict consensus phylogram of section *Limnorchis* based on a parsimony analysis of ITS sequence data

Dr. Song Zhang, Computer Science and Engineering

Modeling

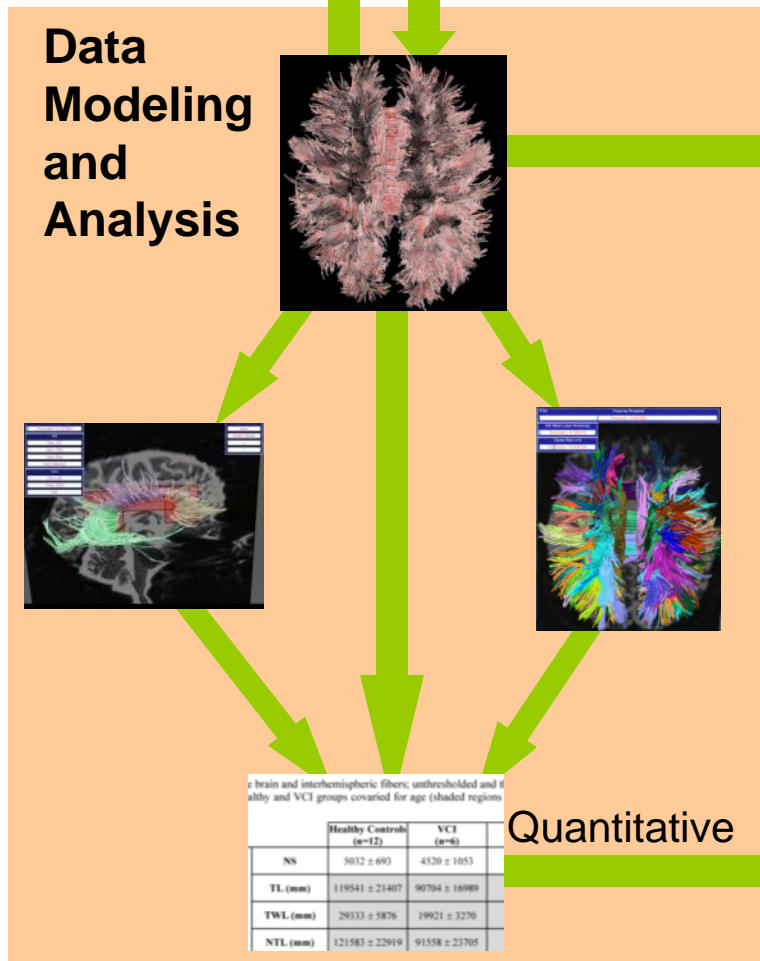
Analysis

Visualization

Application



Diffusion Imaging Visualization and Analysis



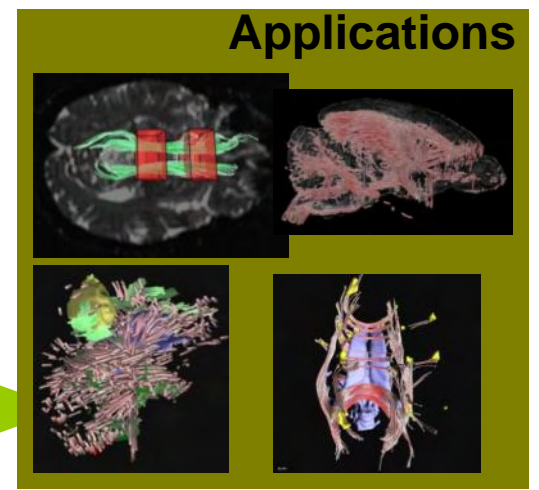
User Study

Qualitative

Quantitative

Brain and interhemispheric fibers; unthresholded and thresholded for healthy and VCI groups covaried for age (shaded regions)

	Healthy Controls (n=12)	VCI (n=6)
NS	5032 ± 693	4520 ± 1053
TL (mm)	119541 ± 21407	90704 ± 16989
TWL (mm)	29333 ± 5876	19921 ± 3270
NTL (mm)	121583 ± 22919	91558 ± 23705



Defect Detection in Liquid Crystals

