NCSA Research Fellows 2016
Ideas Acceleration Workshop

Faculty Research Ideas

National Center for Supercomputing Applications
University of Illinois at Urbana–Champaign

Trish Gregg

Geophysics

Statistical data assimilation strategies to forecast volcanic eruption and mitigate potential disasters

Trish Gregg

Assistant Professor of Geophysics

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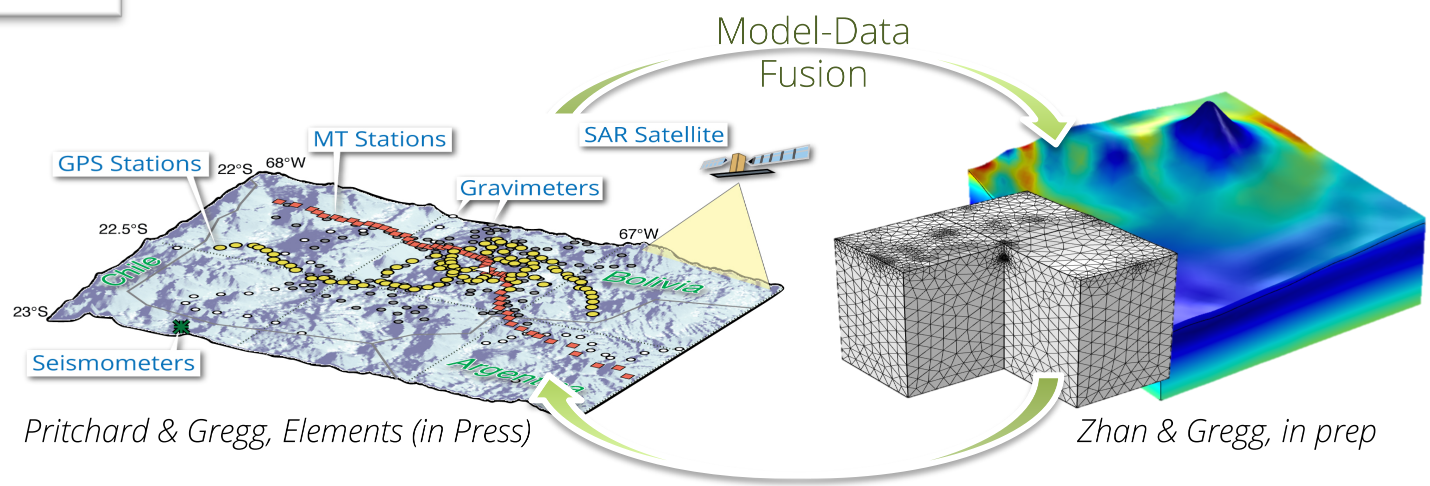
Project Goals:

- Link data with models in near-real time
- Determine eruption precursors
- Develop effective communication strategies



Pritchard & Gregg, Elements (in Press)

Zhan & Gregg, in prep

Project Challenges:

- Computational framework for large-scale data assimilation using Ensemble Kalman Filter
- Thermal fatigue and failure in ductile materials. How are eruptions triggered?
- How to effectively communicate the model forecasts to decision makers and vulnerable populations to mitigate volcano disasters

Interdisciplinary effort that links **Geophysics** data, **Geodynamic** modeling, Mechanical/Material **Engineering**, **Supercomputing** Strategies, **Visualization** strategies, **Sociology** of hazard communication, **Educating** vulnerable populations, and many other areas!

Ange-Therese Akono

Civil and Environmental Engineering

Ange-Therese Akono

Assistant Professor of Civil and Environmental Engineering
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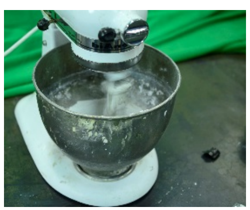
Multi-scale Modeling of Geopolymer Cement for Climate Change Mitigation

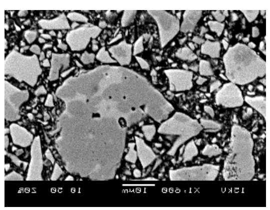
Prof. Ange-Therese Akono, CEE

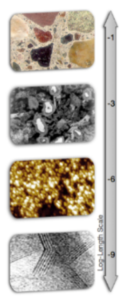
NCSA Thematic Area: Materials and Manufacturing

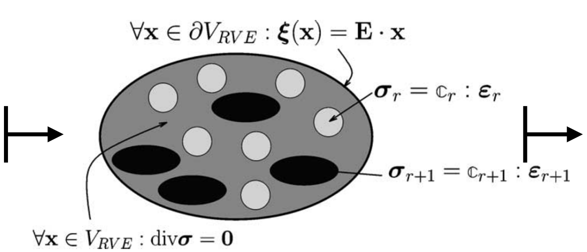
PROJECT SYNOPSIS

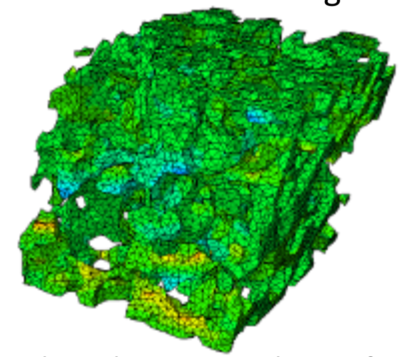
- Geopolymer cement is a low energy construction materials that is strong and fast-curing, with a carbon dioxide footprint much smaller than that of conventional Portland cement
- Micro-poromechanics modeling implemented using Finite Element simulations will pinpoint the origin of mechanical performance from the nanometer to the macroscopic length scale. The integration of Hooke's law, the Hill lemma and Biot's theory, will shed light on the correlation between strength, and stiffness and the microstructure and mix design.
- The fracture behavior will be simulated using a cohesive crack model with bilinear softening.











PROJECT NEEDS

- Computational power to run advanced Finite Elements simulations using a very fine mesh a large number of elements. Parametric studies will analyzed to consider a wide range of configurations
- Power to solve in a timely fashion highly nonlinear problems involving frictionless contact, large deformation, fluid flow following Darcy's law and crack propagation. Use of user subroutines via FORTRAN or Python programming.
- Success will accelerate the discovery of superior construction materials and provide affordable housing to millions of people worldwide.

Les Gasser

GSLIS

Prof. Les Gasser
GSLIS, CS, & CSE
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Simulating Social Systems at Scale

Vision:

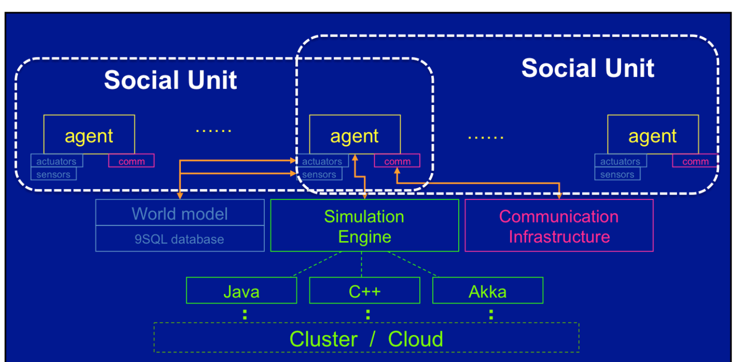
- Cyberinfrastructure for effective, efficient, accessible data-rich scalable simulations of social systems from groups to whole societies , in varying detail.
- Integrated simulation, visualization, data management/analysis
- Solve very hard modeling, computational, and visualization problems

Application, Research, & Education Areas:

- Human/social-environment-technology interactions: disaster; climate change; policy/planning; [Urban] development; Smart cities; migration…
- Basic research: Organization science; Innovation/diffusion; Norms; Information/knowledge/communication in societies & organizations; Language evolution; Security/privacy; Dynamic networks…

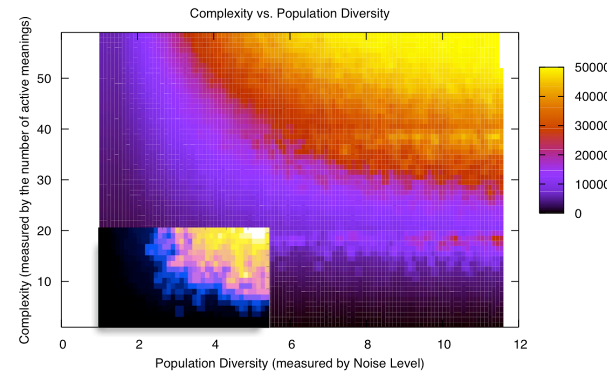
Needs:

- Collaborating data projects
- Visualization
- Application clients
- Infrastructure & scalability expertise



Language convergence

Complexity vs. Population Diversity



Steve Long

Crop Sciences and Plant Biology, IGB

3-D simulations of plant growth at the global scale

Steve Long
Gutgsell Endowed Professor, Department of Crop Sciences and Plant Biology
Faculty, Institute For Genomic Biology
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- **Idea**

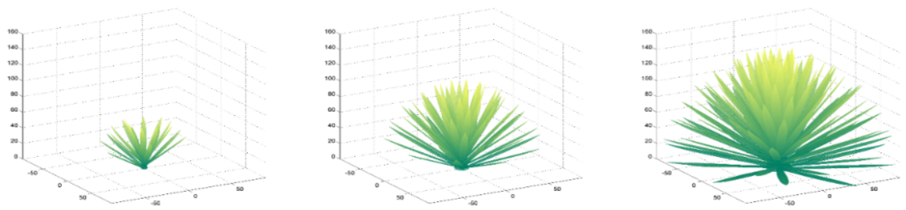
Agave is a potential bioenergy crop, which can potentially be grown in water-limited conditions such as desert (1/3rd of total land area) and can provide an alternative and renewable source of liquid fuel from land which are neither forest, pastures, nor crop land. We have developed a detailed mechanistic and unique growth model that incorporates the mechanisms of response to atmospheric and climatic change. We will now apply to predict where global production potential for bioenergy, greenhouse gas offsets, resource requirements and sustainability, sensitivity to weather variability and future climate change. This is critical information in deciding where this emerging crop would be economically and environmentally sustainable as a bioenergy and bioproduct feedstock.

Problems

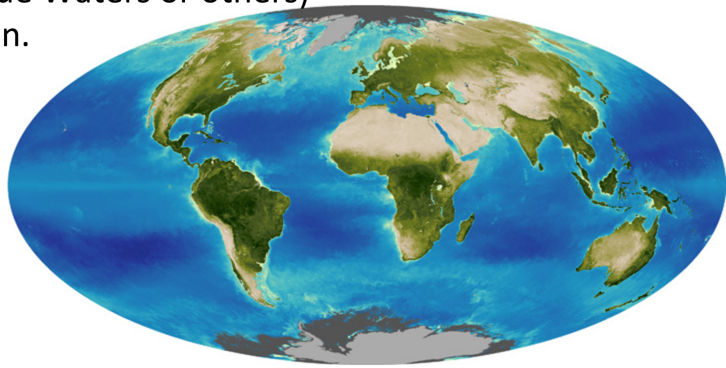
~4550 million hours of simulations (integer node core)

- **Needs**

1. Expertise in GPU programming to accelerate ray tracing component of the model.
2. Computing resources to support numerical integration of the multiple equations describing the capture, conversion of sunlight and its transduction into growth along with fluxes of nutrients into the crop and water through the crop (Blue Waters or others)
3. Spatially high-resolution downscaled global climate change prediction.



Structure of Agave canopy at three different growth stages during growing period of 8 years.



http://earthobservatory.nasa.gov/Features/WorldOfChange/biosphere.php

Dan Miller
Natural Resources and Environmental Sciences

Using Big Data to Advance Understanding of the Long-Term Impacts of Forestry Interventions

Daniel C. Miller, Assistant Professor,
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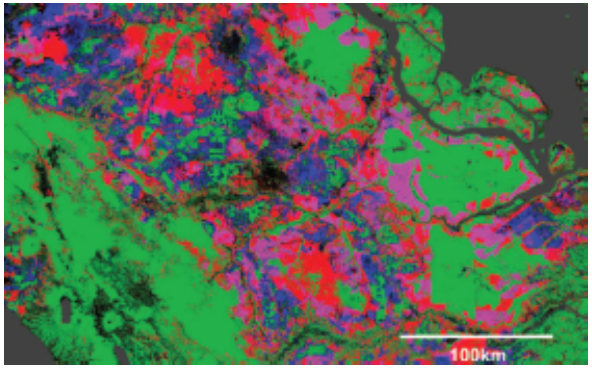
Problem statement: data and methods needed to assess the **long-term impacts** of forestry interventions on **biodiversity, climate change mitigation, economic well-being,** and **food security**.

Objective: advance understanding of how measurement of intermediate targets within project cycles can drive long-term impacts of forest conservation and management.

Approach: use "big data" methods to develop and **empirically validate predictive proxy indicators** (PPIs), measures taken during project or policy implementation capable of predicting longer-term impacts

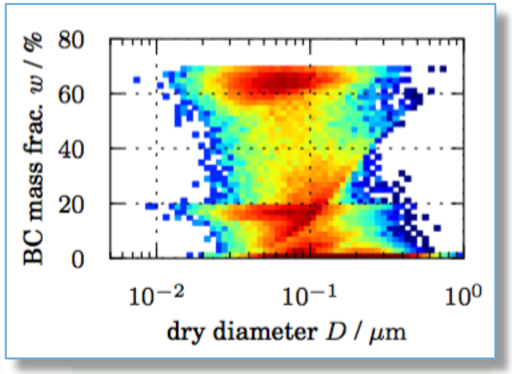


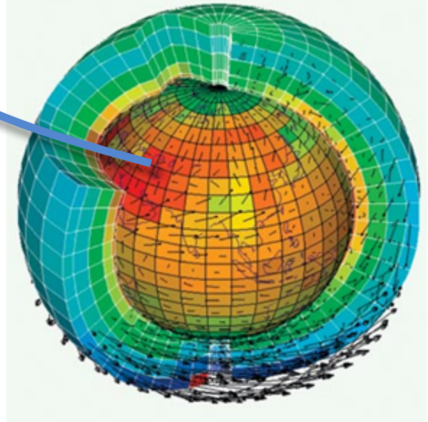
NCSA skills & resources sought:
- Dataset construction based on disparate datasets, incl. remotely sensed, survey, and other "big data"
- Text analysis & computer learning
- Large-scale computing capacity for analysis (Blue Waters)

Matthew West
Mechanical Science & Engineering

Nicole Riemer
Atmospheric Sciences

Learning next-generation aerosol models for global climate simulation





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Problem
Current climate simulations use highly approximate aerosol models with large and unquantified errors (largest current source of uncertainty).

Key Idea
Use new particle-resolved models (PartMC) to accurately resolve aerosol processes, benchmark existing global simulations, and learn improved coarse-grained aerosol and aerosol/cloud models.

Needs
Scaling particle-resolved models to large domain sizes (MPI), machine learning applied to PB-scale data sets (Hadoop).

Matt Browning
Recreation, Sport and Tourism

Ming Kuo
Natural Resources and Environmental Sciences

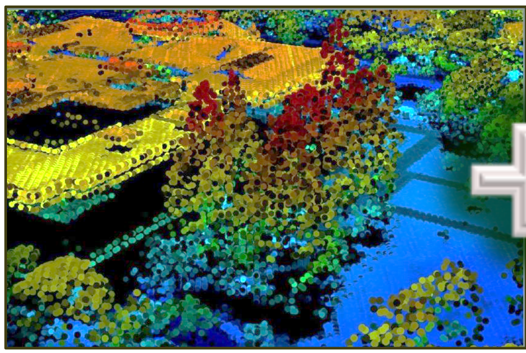
Tying the natural environment to human health with large-scale, longitudinal data from remote sensing and electronic medical records

Matt Browning brownin@illinois.edu
Assistant Professor in Recreation, Sport and Tourism
Affiliated Assistant Professor in Natural Resources and Environmental Sciences

Ming Kuo fekuo@illinois.edu
Associate Professor in Natural Resources and Environmental Sciences
Director of Landscape and Human Health Lab

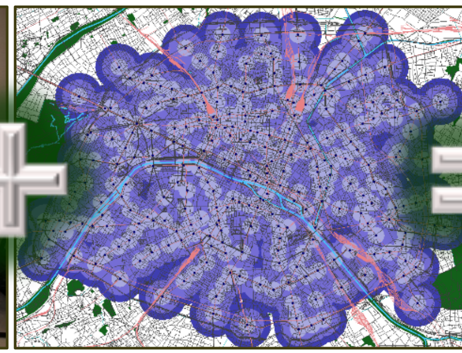
Problem Statement and Research Synopsis

Emerging datasets from medical insurance companies and remote sensing technology provide new opportunities for research on a scale – and with policy implications – not previously possible.



High-resolution LiDAR imagery of the environment around people's homes

Electronic medical records and health care spending from millions of people



GIS buffer analyses of environment around homes, human health, and health care spending

Applications for greenspace development and urban forestry planning, policy

The Need for Supercomputing Power

- Create high-resolution terrain maps of environmental features for 50,000 square miles
- Spatially analyze 3-d maps of environmental features around 4,000,000 points
- Create prediction models for health and spending based on 10 years of data from 2,000,000 people

Michael K. Lim

Business Administration

Optimizing Water Pollution Monitoring System: Regulation policy for curbing water nutrient pollution

Michael K. Lim

Assistant Professor of Business Administration • Computational Science & Engineering (Faculty Affiliate)

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Problem Background

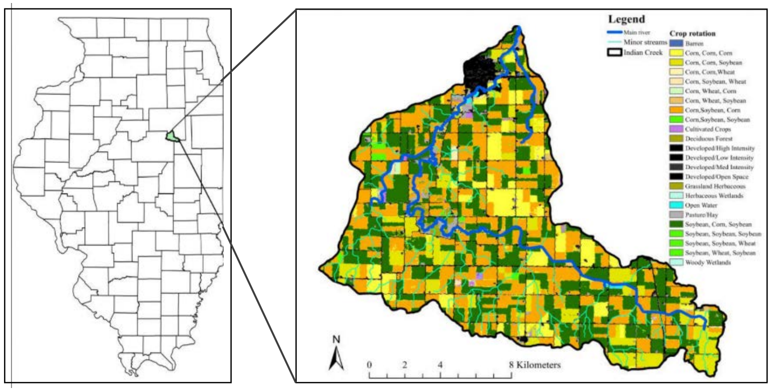
- Current farming practice responsible for massive dead zone (Hypoxic zone) in Gulf of Mexico (fertilizer nutrient N, P flow via Mississippi river)
- Need for efficient governmental regulation policy
- Balanced perspective of economic, environmental, and societal impacts

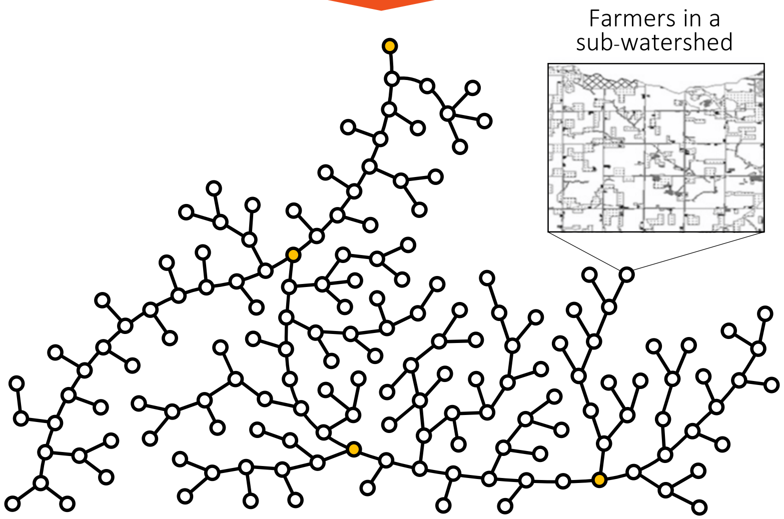
Key Ideas

- <u>Government</u>'s regulation → Network optimization
  - Water network mapping, optimal monitor system location, optimal regulation policy (incentive, penalty, enforcement)
- <u>Farmers</u>' economic behavior → Algorithmic game theory
  - Farming practice (crop choice, fertilizer, filtration buffer zone), Moral Hazard gaming among farmers

Needs

- Computational/Algorithmic challenge (MPEC: Mathematical Programming with Equilibrium constraints)
- Validation of approximation solution method
- Synergetic collaborative research (with on-going NCSA project, *Great Lakes to Gulf* led by Dr. Jong Lee)





Example: Hydrological water network of Indian Creek watershed

Lei Tian
Agricultural and Biological Engineering

Liujun Li
Agricultural and Biological Engineering

CyberGIS-enabled Ag big data analytics

PI: Lei Tian, Liujun Li, Co-PI: Shaowen Wang
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http://abe-research.illinois.edu/remote-sensing/index.html

- **State-of-the-art Ag remote sensing data and cloud computing prototyping**
- **Data-mining-driven Tempo-Spatial modeling beyond horizontally and historically**
- **Real-time site-specific precision farming decision making enabling**