NIMBioS and Computational Science: Fostering Research and Education at the Interface of Mathematics and Biology

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Theory and Biology: one recent view

1. Are there still new life forms to be discovered?
2. What role does life play in the metabolism of planet Earth?
3. How do cells really work?
4. What are the engineering principles of life?
5. What is the information that defines and sustains life?
6. What determines how organisms behave in their worlds?
7. How much can we tell about the past and predict about the future by studying life on earth today?

The Role of Theory in Advancing 21st-Century Biology: Catalyzing Transformative Research (NRC, 2008)
Linkages between different species (e.g. vector-borne disease), environmental and anthropogenic factors require a systems perspective to evaluate the nature of the linkages. This could benefit from the new methods for multi-scale models and analysis which is a very active area of computational science.
NIMBioS Vision

- Foster new collaborative efforts to investigate fundamental and applied questions arising in biology using appropriate mathematical and computational methods
- Enhance the essential human capacity to analyze complex biological questions and develop necessary new mathematics
- Encourage broader public appreciation of the unity of science and mathematics.
General Methods

• Choosing fundamental problems that will benefit from cross-disciplinary collaborations.
• Choosing applied problems of sufficient general interest to be readily extended beyond an initial region/ organism/ system.
• Building appropriate collaborations to address these fundamental and applied problems.
• Developing education and outreach opportunities to diversify participation in these collaborations at all levels.
Specific Methods

• Focused research projects (Working Groups) to build collaboration among diverse communities.

• Building collaborations through more open-ended general problems, addressed through multiple approaches (Investigative Workshops).

• Skill and methods-based programs (Tutorials) that foster a broader understanding of potential applications of modern math and computational science in biology.

• An expansive set of education-linked-to-research endeavors from elementary through post-doctoral level that provide diverse opportunities at the math/biology interface.
Post-doctoral Fellows

- Post-docs are independent researchers chosen based upon a proposal that fits NIMBioS opportunities.
- Each post-doc is assigned two mentors, one from mathematical/computational sciences and one from biology.
- Post-docs are given the opportunity to teach regular UT classes and to make short term visits to our partner Minority Serving Institutions.

Sabbatical Fellows - we offer a limited number of these for visits longer than a month

Short-term Visitors - for periods of a few days to less than a month to use our facilities or collaborate.
NIMBioS participants:
284 different institutions,
46 states,
28 countries
Working Groups and Investigative Workshops

**Working Groups:**
- Coalitions and Alliances.
- Intragenomic Conflict.
- Feral Swine / Pseudo-rabies in Great Smoky Mountains National Park.
- Biological Problems using Binary Matrices.
- Synthesizing and Predicting Infectious Disease while Accounting for Endogenous Risk (SPIDER).
- Integrating Functional and Evolutionary Dynamics at Multiple Scales.
- Population and Community Ecology Consequences of Intraspecific Niche Variation.
- Cross-Topology Registration.
- Modeling Bovine Tuberculosis.
- Synthesizing Predictive Modeling of Forest Insect Dynamics Across Spatial and Temporal Scales.
- Food Web Dynamics.
- Multi-scale Analysis of Cortical Networks.
- Species Delimitation.
- Gene Tree Reconciliation.
- Multiscale Modeling of the Life Cycle of *Toxoplasma gondii*.

**Investigative Workshops:**
- Modeling White Nose Syndrome in Bats at the Individual and Colony Levels: Epizootiology and Management.
- Modeling the Impact of Cattle Movements on Transmission Dynamics of Bovine Tuberculosis in the United States.
- New Strategies for the Black Box: Identifying mathematical tools for elucidating plant-soil interactions.
- Optimal Control and Optimization of Individual-based and Agent-based Models.
- Modeling *Toxoplasma gondii*.
- Modeling Reef Ecosystems.
- Modeling Wildlife and Virus Zoonoses.
- Solid Tumor Modeling (and poster session).
- Modeling Infectious Disease.
- Synchrony in Biological Systems Across Scales.
- Marlaria Modeling and Control.
- Modeling Johne’s Disease.
- Modeling Metabolism and Body Weight Regulation.
- Modeling Renal Hemodynamics.
Recent and Upcoming Workshops

Individual-based Ecology of Microbes: Observations and Modeling (June 8-10)
Malaria Modeling and Control (June 15-17)
Investigating Johne's Disease Epidemiology and Immunology through Mathematical Modeling (July 6-8)
Mathematical Models of Metabolism and Body Weight Regulation (July 12-15)
Modeling Renal Hemodynamics (Aug 1-3)
Modeling Intracellular Movements (Oct 24-26)
Modeling Free-Roaming Cats and Rabies (Nov 9-11)
Modeling Social Complexity (Feb 6-8, 2012)
Environmental Modeling

Data sources
- GIS map layers (Vegetation, hydrology, elevation), Weather, Roads, Species densities

Species densities
- Animal telemetry
- Physical conditions

Monitoring

Management input
- Harvest regulation
- Water control
- Reserve design

Models
- Statistical Differential equations
- Matrix
- Agent-based

Evaluation/Analysis
- Visualization, corroboration, sensitivity, uncertainty

Simulation
- Matlab, C++, Distributed, Parallel
HPC Opportunities at NIMBioS:

- Tutorials on high performance computing for biologists
- HPC Specialist and scientific coding experts in biology to assist participants in use of NIMBioS 128-core cluster
- Priority access for NIMBioS participants to Kraken and Nautilus
HPC Resources at NIMBioS

- 128 core cluster composed of Quad core AMD opteron Processor 2376.
- 24 GB of memory is available per node
- Infiniband interconnect
- 5 Terabyte storage RAID
- MATLAB, R, MPI, GCC, Portland Group
- ROCKS implemented on CentOS
Opportunities

- The NIMBioS Cluster small size makes it a starting point to begin development in preparation for larger Clusters.
- Usage that fit within the NIMBioS mandate are welcome to apply for access.
- Contact: Eric Carr carr@nimbios.org
R is a major development tool in the Biology community

- Success is often found through many serial runs of R application using array submissions.
- Multiple core and parallel runs scaling is still a work in progress.
- Memory management for very large problems can also be a challenge.
- RDAV on Nautilus have been working on some of these implementation issues.
Research Experience for Undergraduates and Veterinary Students

- Opportunities to work with researchers on relevant problems.
- Leverage resources and knowledge at NIMBioS
Postdoc: Xavier Thibert-Plante
Biodiversification in a changing environment

Ecological speciation on heterogeneous environments

"Understanding the processes underlying biodiversity can help direct our actions to minimize our impact on living organisms."
“Our general hope is that we may identify some means of influencing the outcomes of the WNS (White-Nose Syndrome) outbreak so that bats remain abundant contributors to ecological communities, but this is more of a management goal than a scientific one.”
Working Group
Feral Swine / Pseudorabies

QUESTION 1: Optimal balance of control vs. surveillance?

QUESTION 2: Where to focus control to minimize chance of transmission to livestock?
Question 3: Predicting feral swine range expansion in southeastern States (implications for Foreign Animal Disease containment)?

Raw data for Arkansas

Predicted expansion at annual intervals

Stream-buffered diffusion model
Review Paper: approaches to predictive modeling of disease at the wildlife/livestock interface

Modeling Disease in Feral Hogs:

25 published models

(11 FMD, 8 CSF, 2 PRV, 4 others)

Model Type

Conceptual 2

Statistical non-dynamic (GLM, etc) 8

Non-spatial deterministic (ODE) 4

Non-spatial stochastic 2

Reaction-diffusion (PDE) 2

Cellular automata 3

Geographic automata 4
HPC Tutorials at NIMBioS
http://nimbios.org/tutorials

• Migration from the Desktop: HPC application of R and other codes for biological research
• High Performance Computing for Phylogenetics
• High-Performance Computing for Computational Science Professionals Collaborating with Biologists
Welcome to NIMBioS

At NIMBioS, the talents of top researchers from around the world collaborate across disciplinary boundaries to find creative solutions to today’s complex biological problems. Our Education and Outreach Program focuses on the interface between mathematics and biology and promotes cross-disciplinary approaches to science for learners of all ages.

The Dynamics of Disease

Folashade Agusto is a NIMBioS postdoctoral fellow who studies the transmission dynamics of human and animal infectious diseases. Click here to view the video.

The Evolution of Biodiversity

The rate of climate change is happening so fast that many species cannot adapt quickly enough and risk extinction. Dr. Thibert-Plante studies the interaction between ecological and evolutionary forces and their impact in

NSF Funding Opportunity

A new opportunity has been announced for support of research at the interface of the biological and either the mathematical or physical sciences. The Research Coordination Networks Physical/Life Sciences Interface track (RCN-PLS) is seeking proposals. Application deadline: August 16, 2010. For more information and how to apply, click here.
Songwriter-in-Residence Program

Objective: The National Institute for Mathematical and Biological Synthesis, in conjunction with the Univ. of Tennessee’s James R. Cox Endowment Fund, is sponsoring a Songwriter-in-Residence Program to encourage the creation and production of songs involving ideas of modern biology and the lives of scientists who pursue research in biology. The Songwriter-in-Residence Program supports a four-week long residency of singer-songwriters at NIMBioS. Those selected for the program will be required to be on-site at the NIMBioS offices a minimum of three days per week during the month-long residency. While at NIMBioS, the Songwriter-in-Residence will have the opportunity to interact with resident and visiting scientists at NIMBioS and attend workshops, tutorials and other NIMBioS events. Up to five songwriters-in-residence will be supported from November 2010 through June 2011; one will be in residence at a time. By the end of the residency, the songwriters will be expected to have written, composed and produced several songs. Copyrights to the songs will be shared among the creator, any scientist(s) involved in the songwriting process, and the Univ. of Tennessee. Songwriters-in-Residence will be paid a stipend of $3,000 for the month-long residency.

Songwriters-in-Residence are chosen based on their ability and experience to compose, produce, and perform live songs; their interest in making connections in music between general audiences and science; and their experience touring.

Applications are now closed.

Click here to read more about the 2009 BioSongs project, which inspired the Songwriter-in-Residence Program.

Jay Clark
Songwriter-in-Residence: January 2011

Americana Musician Jay Clark Headlines January Residency Draws to a Close With Mini-Concert

See NIMBioS.org for more information