



Space and Control in Natural Systems

Louis J. Gross

National Institute for Mathematical and Biological
Synthesis

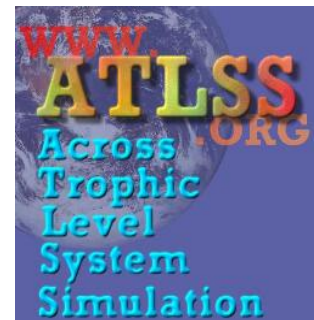
Departments of Ecology and Evolutionary
Biology and Mathematics

University of Tennessee

Supported by NSF Awards DEB-0219269, DMS-0211991, IIS-0427471,
EF-0832858



ATLSS.org



NIMBioS.org

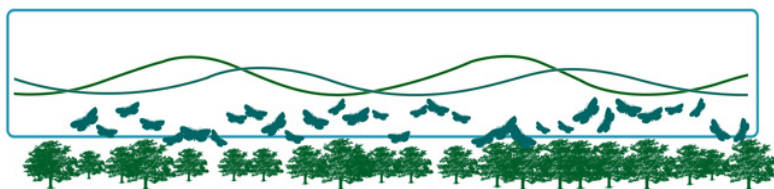




- Foster new collaborative efforts to investigate fundamental and applied questions arising in biology using appropriate mathematical and computational methods
- Enhance the essential human capacity to analyze complex biological questions and develop necessary new mathematics
- Encourage broader public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

Some NIMBioS Activities

- 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.
- **Postdoctoral and Sabbatical Fellowships**
- **Short-term Visitors**
- A summer **Research Experience for Undergraduates** program with teams of math and biology students.



$$\frac{dQ}{dt} = f(Q, M)$$

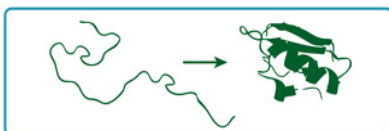
$$\frac{dM}{dt} = g(Q, M)$$

POPULATION DYNAMICS



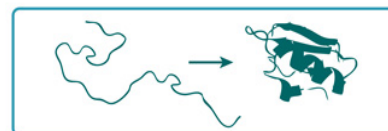
$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial t^2}$$

CELLULAR DIFFUSION



$$V = \frac{V_{\max}[s]}{k_m + [s]}$$

ENZYME KINETICS



$$\Delta p = sp(1-p)$$

GENETIC VARIANCE



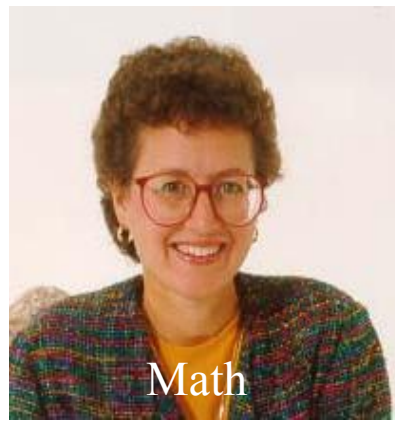
Overview

- Background on natural resource management
- Everglades restoration and ATLSS (Across Trophic Level System Simulation)
- Raccoon rabies and spatial vaccination
- Wildfire control
- Individual-based models for spatial management of black bears
- Optimal control for agent-based models
- *Control of tick-borne disease*
- *Invasive species management*
 - *Optimal control for generic focus/satellite spread*
 - *Spatially-explicit management of Old World Climbing Fern*
- Some lessons

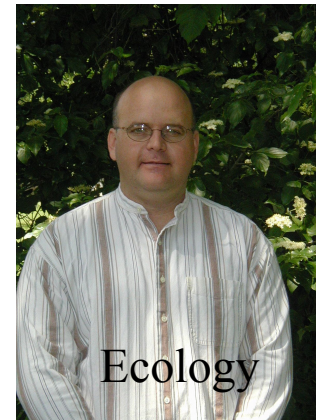




Computer Science/ Ecology



Math



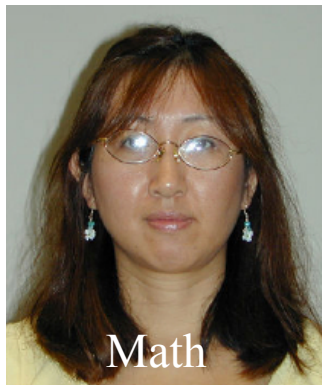
Ecology



Computer Science



Math



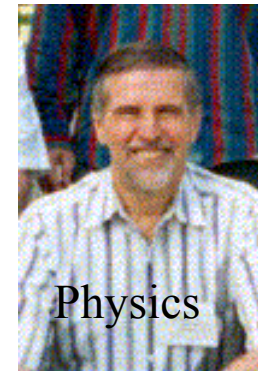
Math



Math/ Ecology



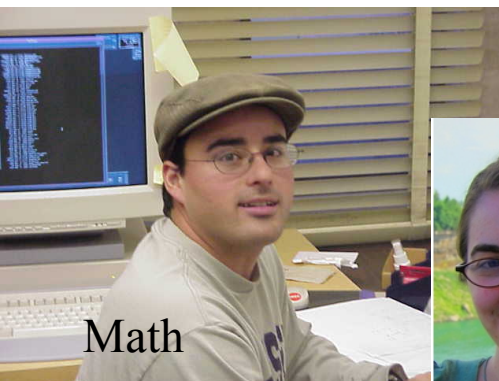
Computer Science



Physics



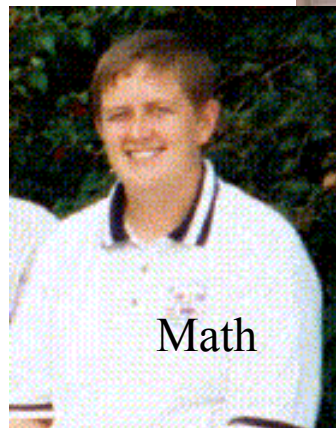
Computer Science



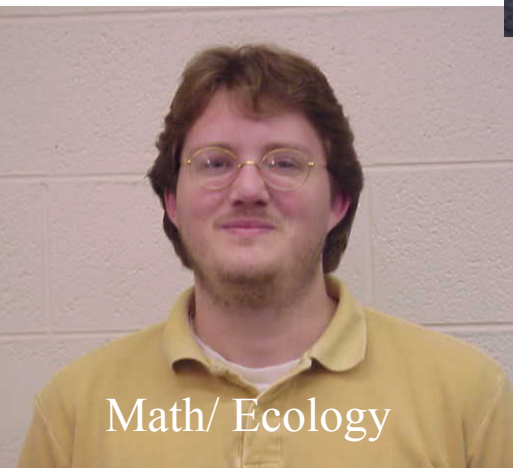
Math



Math



Math



Math/ Ecology



Ecology

Problems in Natural Resource Management

- Harvest management
- Wildlife management including hunting regulations and preserve design
- Water regulation
- Invasive species management
- Disease control
- Fire management
- Agricultural systems management
- Biodiversity and conservation planning

Computational Science for Natural Resource Management

Recent advances in miniaturization, computing power, remote sensing, and modeling are revolutionizing the science of natural resource management. But these advances also bring many challenges. This article highlights some key problems in resource management that represent opportunities for computer scientists and engineers in search of challenging practical problems.

Natural resource managers must balance the needs of complex, dynamic ecological systems with the competing demands of social, political, and commercial stakeholders. Natural resources include wildlife and habitats that provide significant recreational (such as hiking, fishing, and hunting), economic (such as timber harvesting and gene mining), aesthetic (such as scenic landscapes), or functional (such as nutrient retention and flood control) value. The ecological and environmental processes governing functioning ecosystems are difficult to manage because they involve multiple components that operate over broadly disparate temporal and spatial scales. To manage the components of natural reserves, biologists have traditionally relied on rule-of-thumb strategies based largely on what worked in the past.

Model-driven strategies have largely replaced the data-driven approach. Model-driven strategies attempt to project system behavior under alternative management scenarios. Such models are fre-

quently wedded to emerging technologies for data collection and monitoring, such as real-time remote sensing and GPS. But while these advances greatly improve ecological information's temporal and spatial resolution, they also generate large volumes of data. This flood of information increases the demand for efficient data analysis, storage, and communication. At the same time, the evolution of approaches based on disparate technologies and computing platforms complicates the sharing and integration of data from different sources.

As resource managers struggle to cope with these challenges, they've turned to computational science for solutions. The rapid advance of software and architectures designed to exploit improvements in networking, interoperability, and data management has revolutionized natural resource management. The recent changes to natural resource management in many ways mirror those of molecular biology, whose dependence on high-performance computing is well known. For example, researchers have expressed biochemical network models as stochastic Petri nets, a mathematical formalism developed in computer science.¹ Another example is the use of high-performance algorithms to improve the computationally intense sequence comparisons used in molecular phylogenetics.²

As a consequence of computerization, management programs have grown rapidly in size, com-

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AND MICHAEL W. BERRY
University of Tennessee

What is challenging about natural resource management?

- Involves complex interactions between humans and natural systems
- Often includes multiple scales of space and time

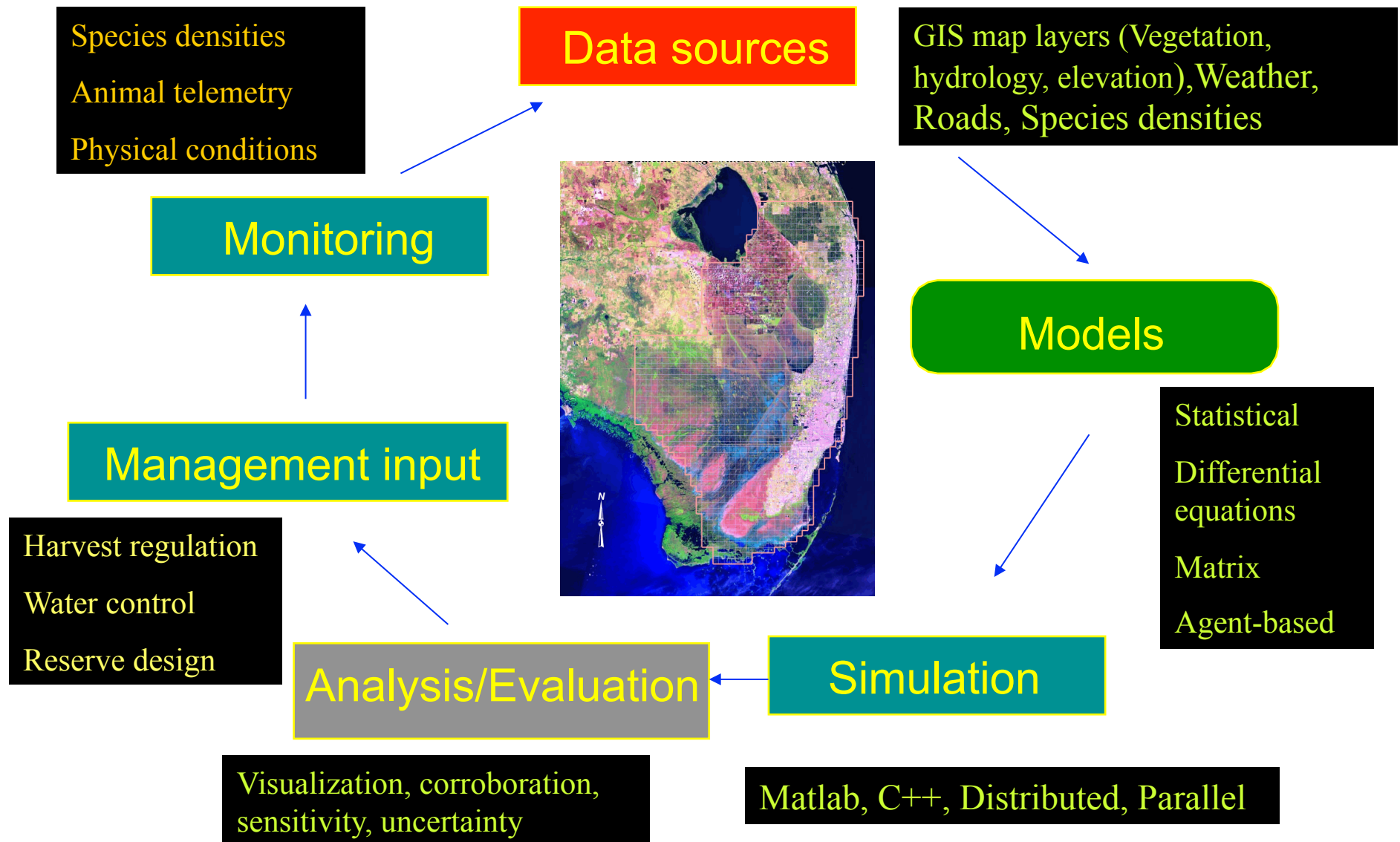


- Multiple stakeholders with differing objectives
- Monetary consequences can be considerable

How can mathematics and modeling assist in solving problems in resource management?

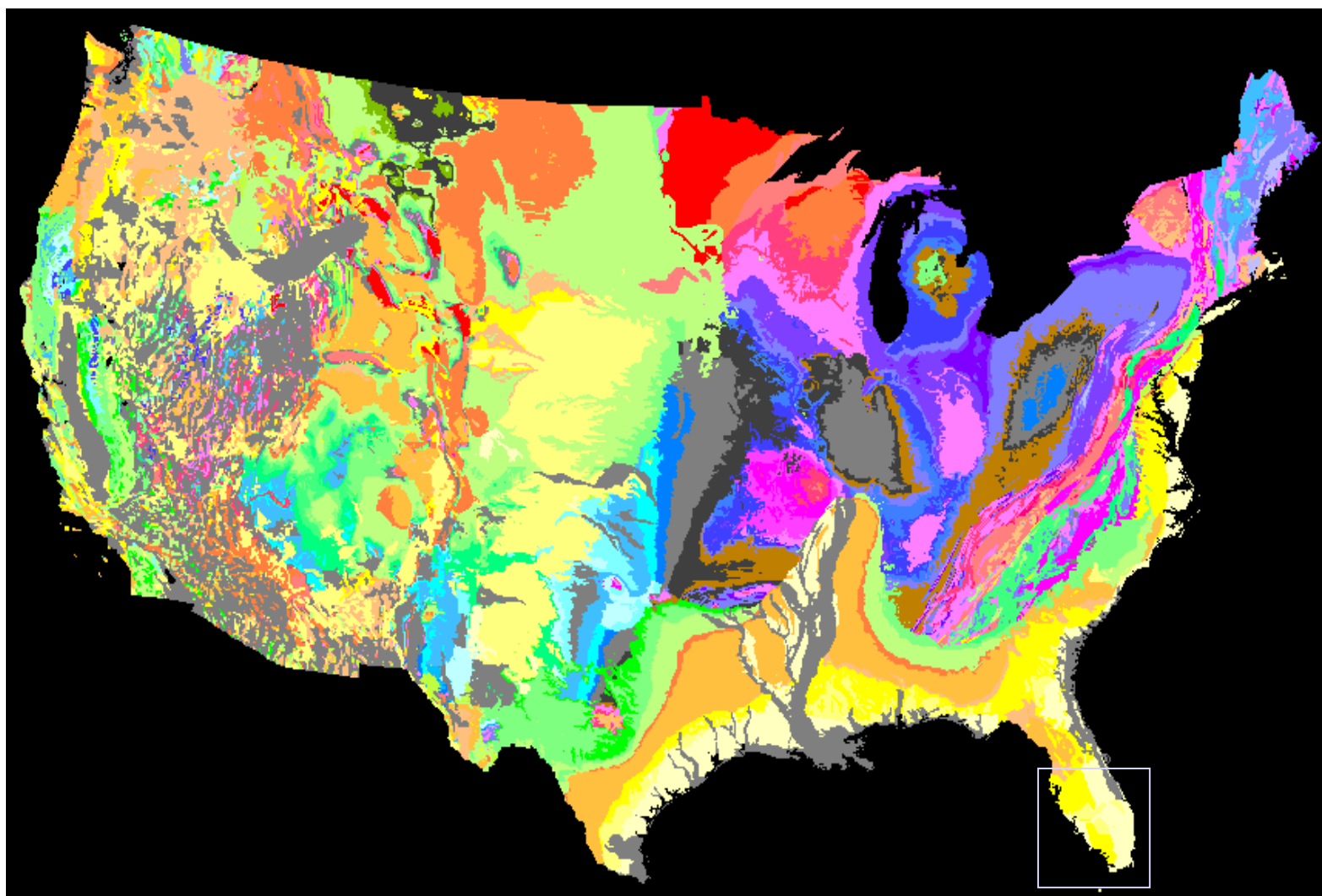
- Provide tools to project dynamic response of systems to alternative management
- Estimate the “best” way to manage systems - optimal control
- Provide means to account for spatial changes in systems and link models with geographic information systems (GIS) and decision support tools that natural system managers and policy makers need.
- Consider methods to account for multiple criteria and differing opinions of the variety of stakeholders

Environmental Modeling



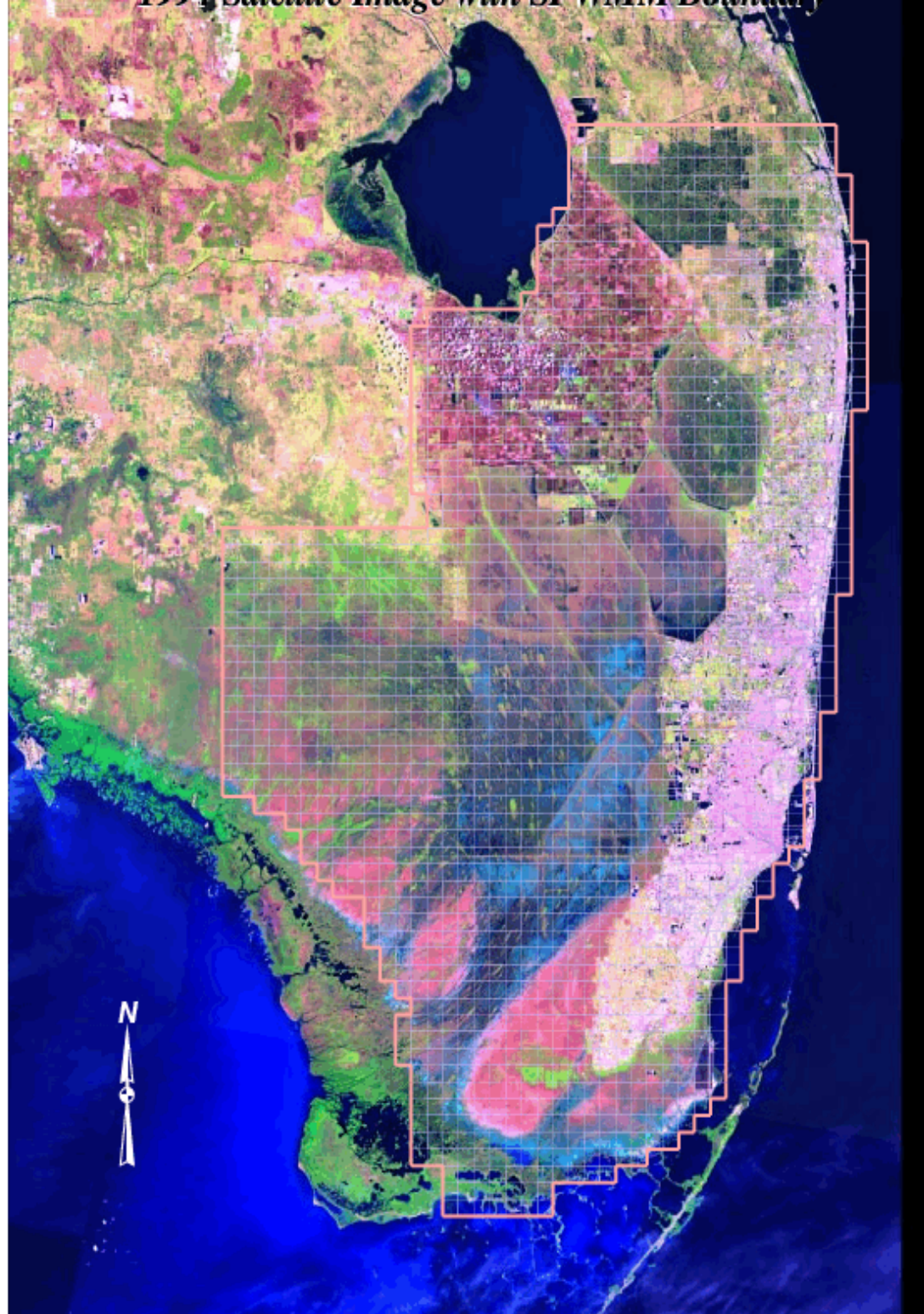
Modeling and optimization

- *Scenario analysis* provides a method to compare sets of assumed inputs.
- *Optimal control* provides a method to decide what is “best” given an objective function, constraints, and dynamical system
- *Sensitivity analysis* provides a method to determine systematically the model response to local changes in assumptions (e.g. parameters)
- *Uncertainty analysis* provides a method to determine model response (generally not systematically) to alternative model structures or non-local changes in assumptions (e.g. Latin Hypercube sampling approaches)
- For many models for management application, it is *ranking* of alternatives that matters, so a relative assessment procedure may be useful (e.g. see Fuller, M.M., L.J. Gross, S.M. Duke-Sylvester and M. Palmer. 2008. Testing the robustness of management decisions to uncertainty: Everglades restoration scenarios. *Ecological Applications* **18**(3):711-723)





1994 Satellite Image with EI Warm Boundary

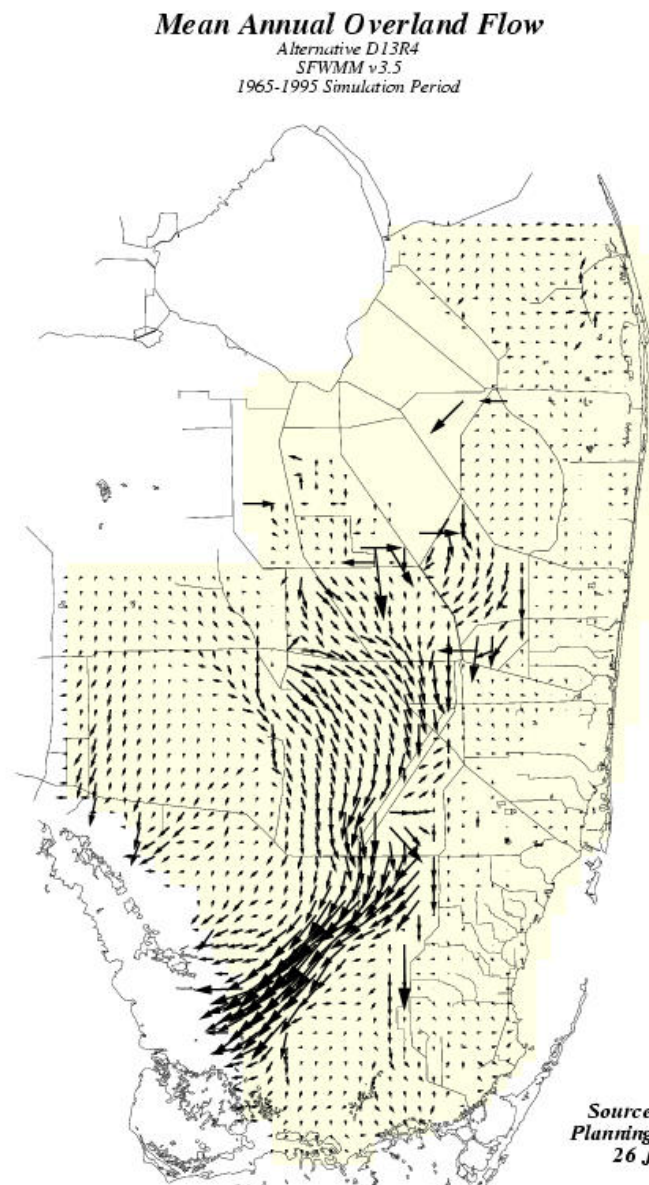
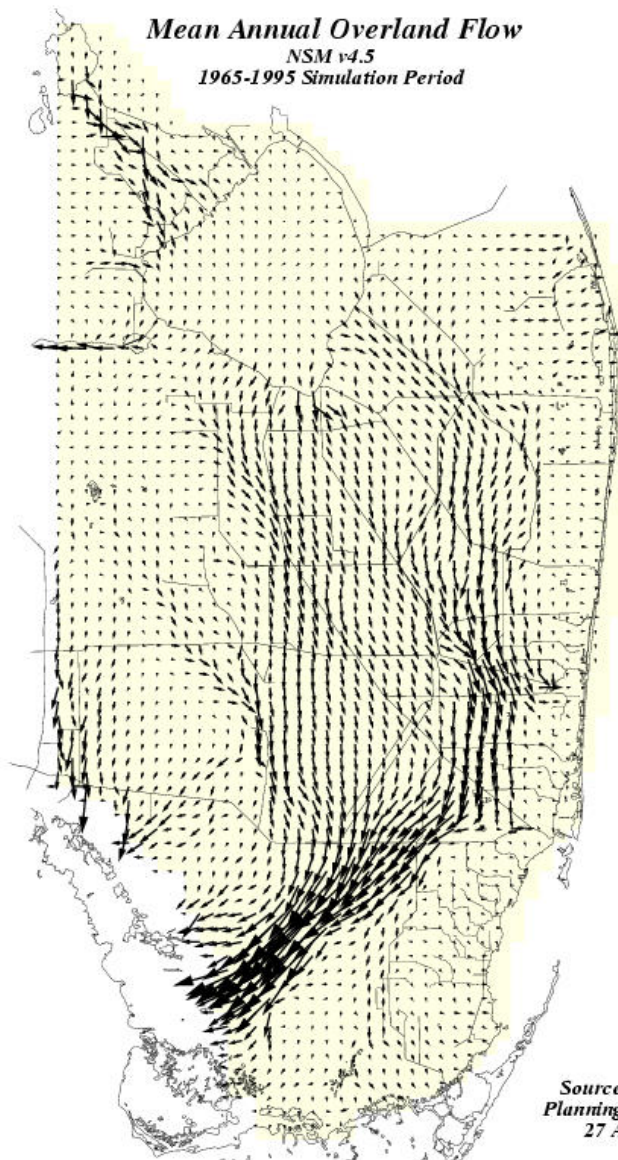


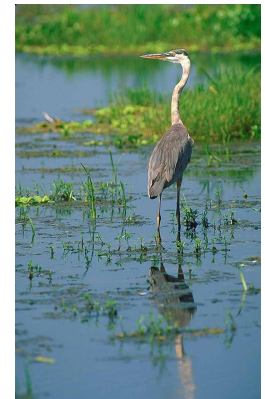
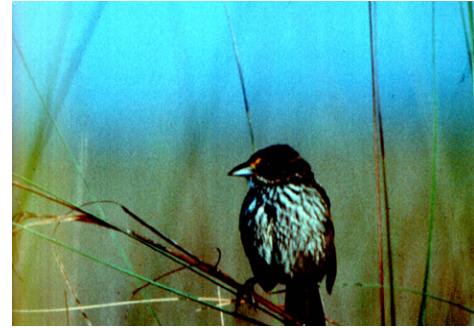
Wet Season:
May-October



Dry Season:
November-April



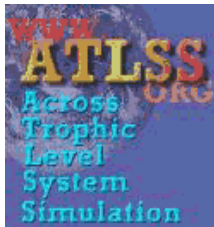




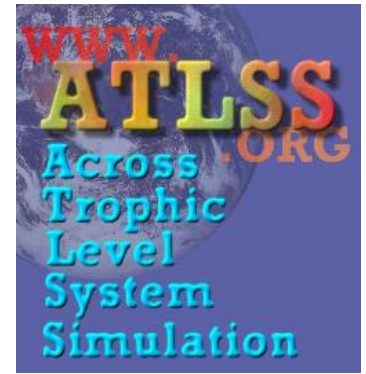
Everglades natural system management requires decisions on short time periods about what water flows to allow where and over longer planning horizons how to modify the control structures to allow for appropriate controls to be applied.

This is very difficult!

- The control objectives are unclear and differ with different stakeholders.**
- Natural system components are poorly understood.**
- The scales of operation of the physical system models are coarse.**



So what have we done?



Developed a multimodel (ATLSS - Across Trophic Level System Simulation) to link the physical and biotic components.

Compare the dynamic impacts of alternative hydrologic plans on various biotic components spatially.

Let different stakeholders make their own assessments of the appropriate ranking of alternatives.

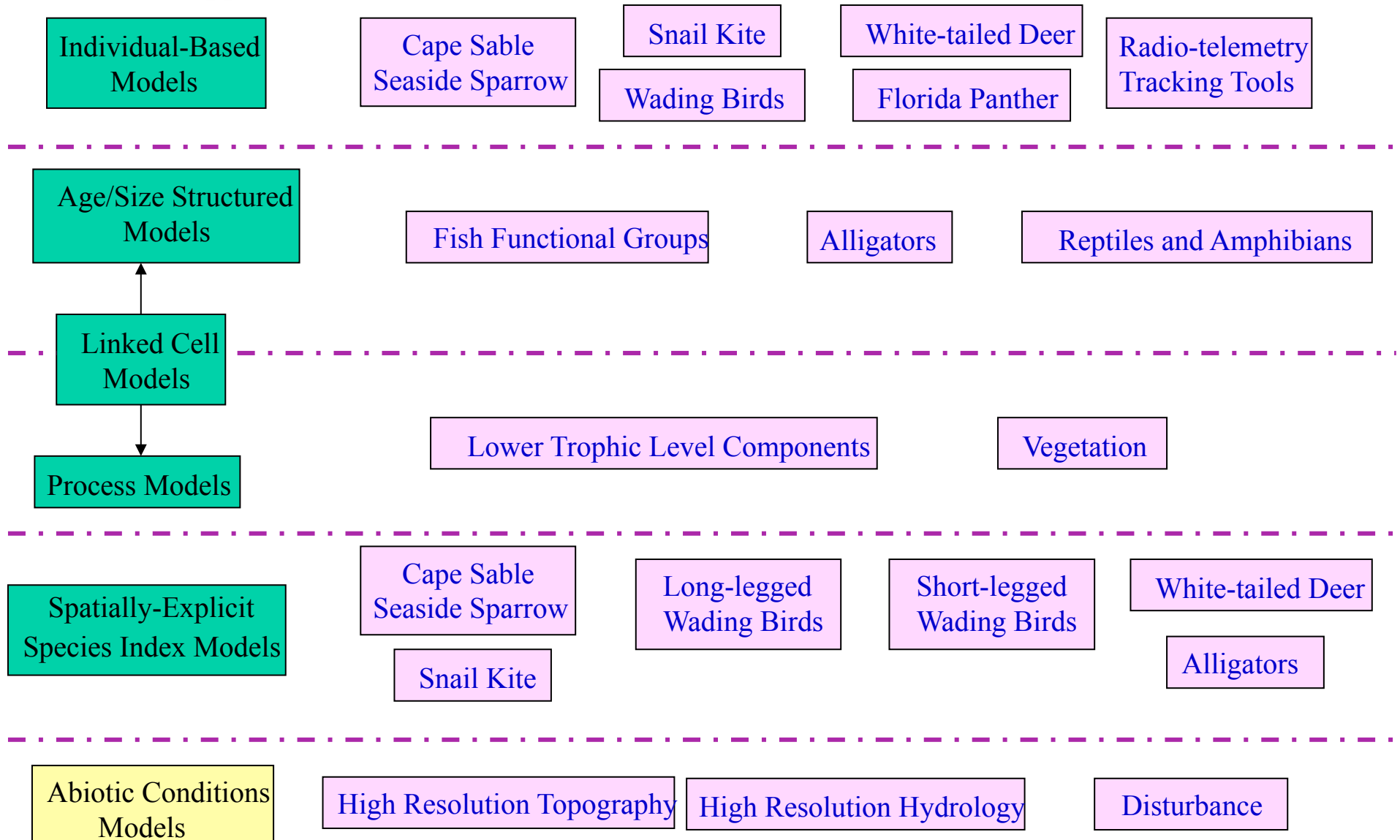


<http://atlss.org>

ATLSS STRUCTURE

Across Trophic Level System Simulation

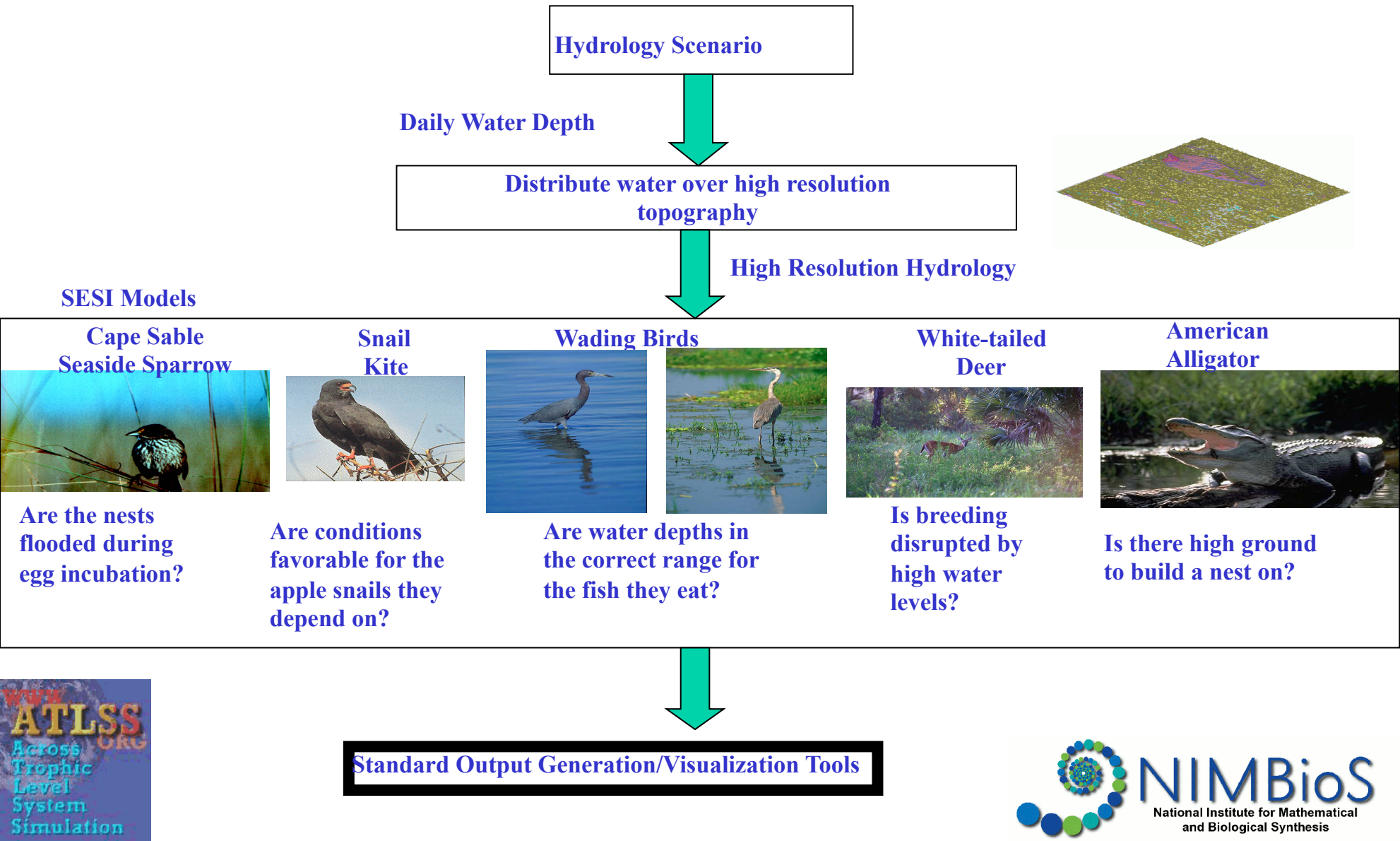
Model Type

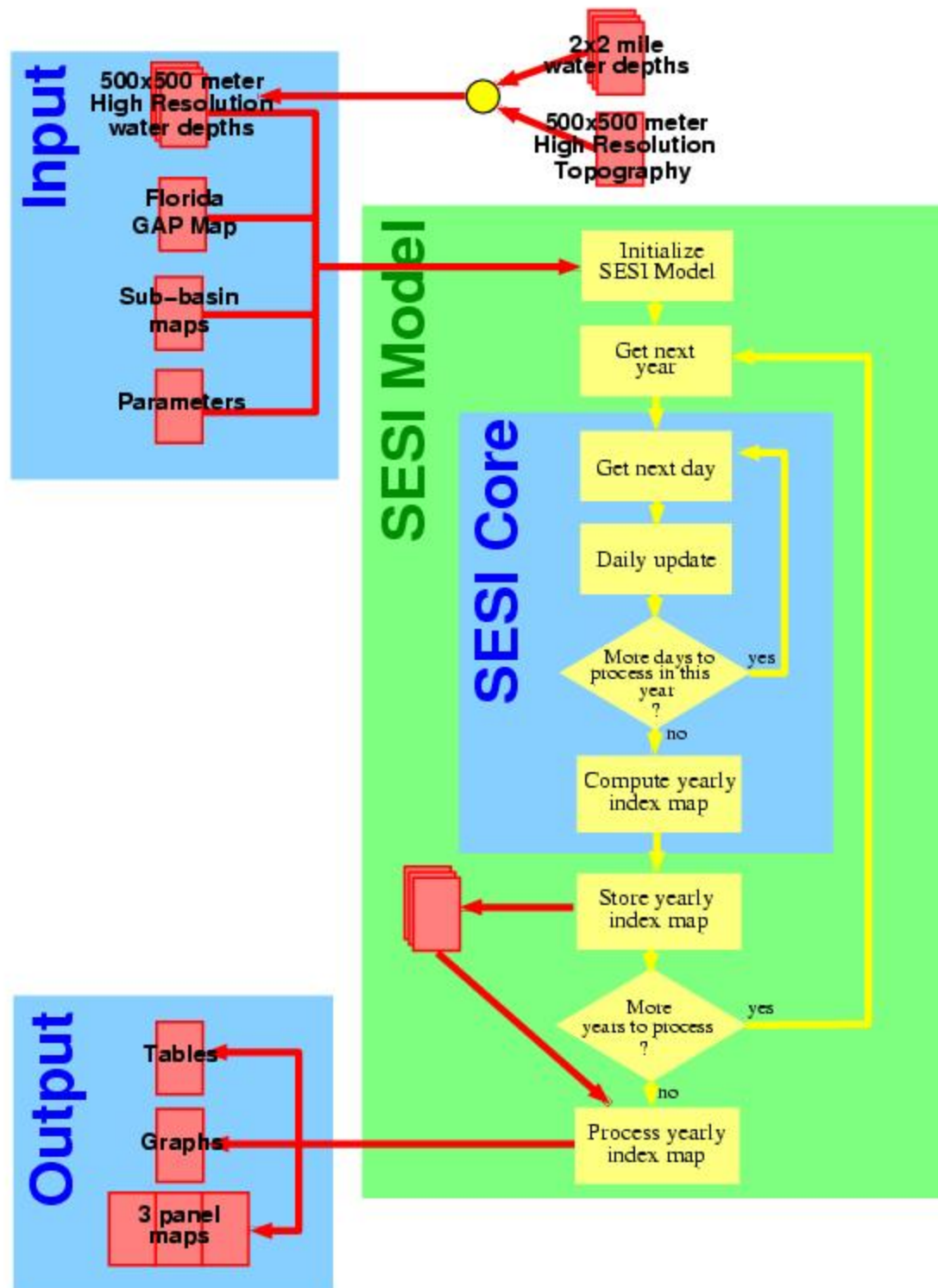


ATLSS SESI Models

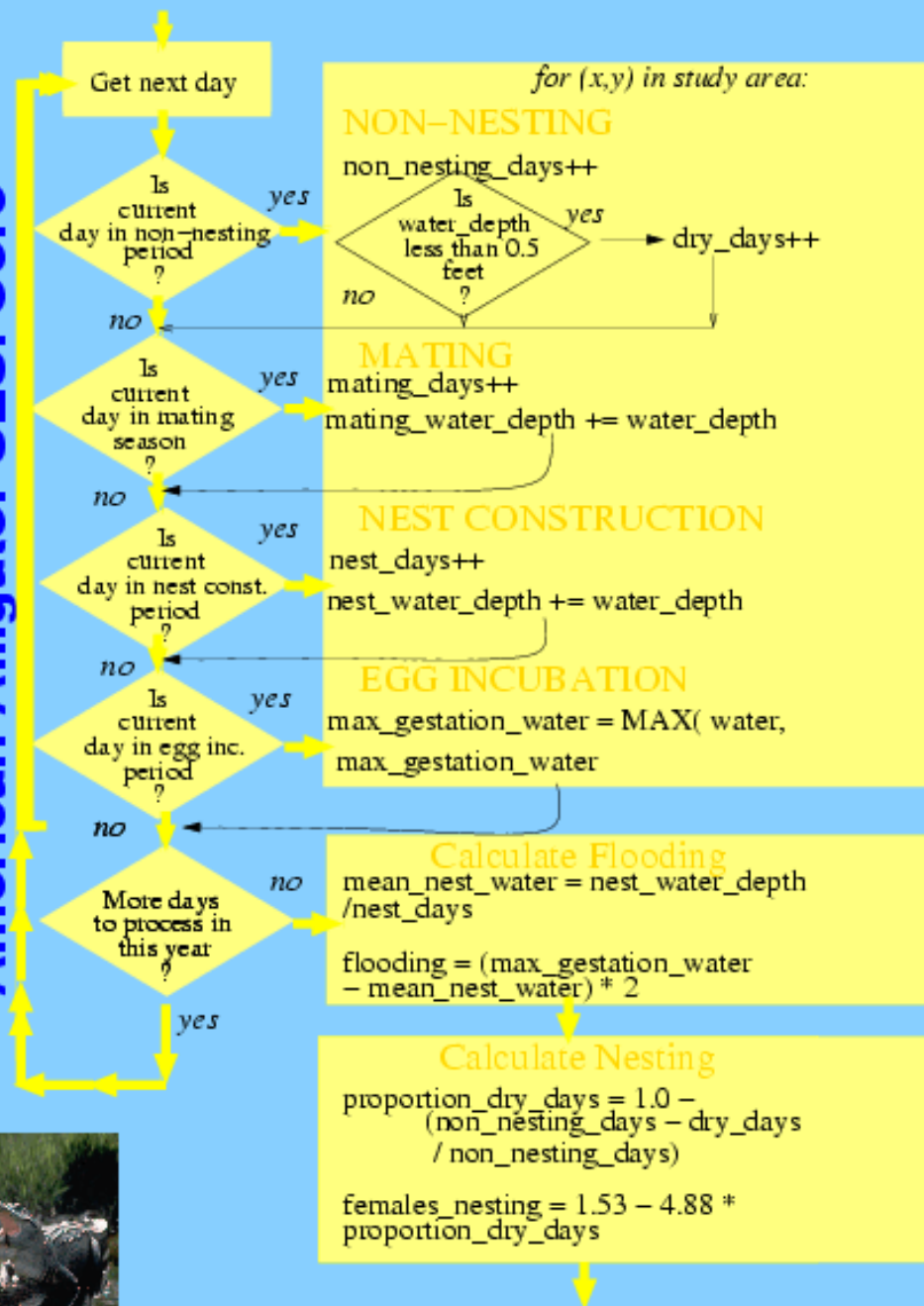
Implement and Execute the Models for a Hydrology Scenario

Objectives: Integrate SESI components into a cohesive computational framework and apply the models to a hydrology scenario.





American Alligator SESI Core

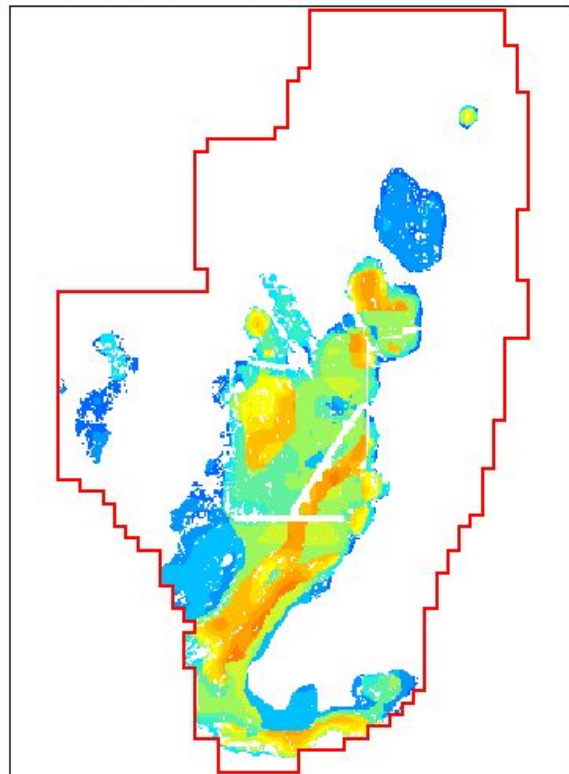


Assessment of the Effects of Proposed Water Regimes

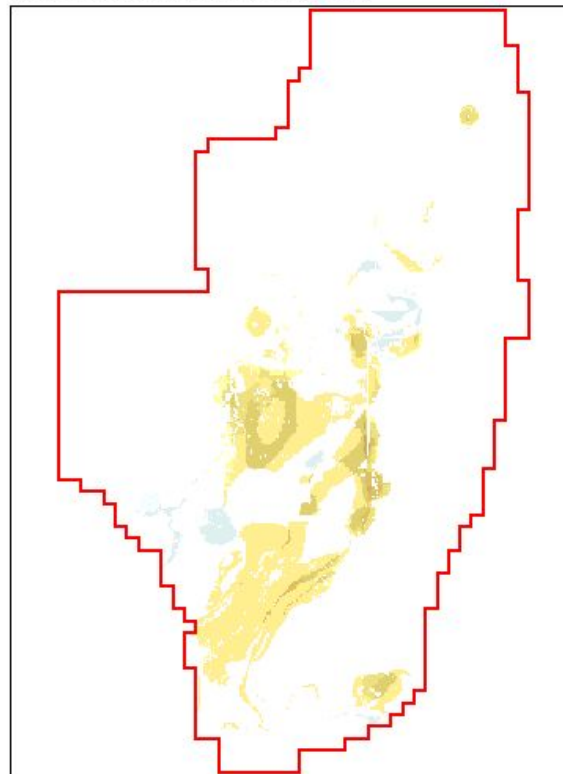
Baseline: F2050 WL1975 versus Alternative: D13R WL1975

Map printed October 10, 2001

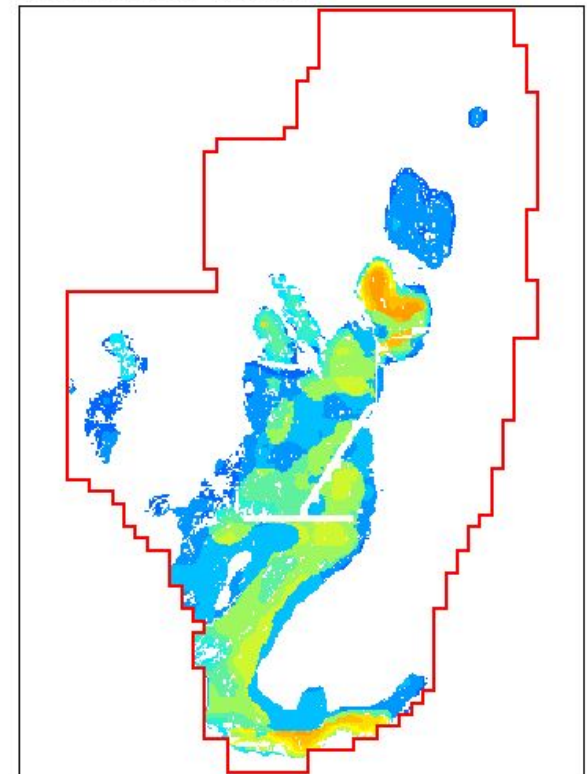
Alternative: D13R WL1975



F2050-D13R WLWL 1975:1975



Baseline: F2050 WL1975



Project Area



Scale: 1 : 4124008

20 0 20 40 60 80 Kilometers



Universal Transverse Mercator (UTM)
NAD83
Zone 17

ANALYSIS TYPE: - Comparison Analysis
AUTHOR: - NWRC
DATE: - Wed Oct 10 15:53:59 2001

>>> BASELINE SCENARIO
TIME INTERVAL: - 1975 (1 year)
HYDROLOGIC REGIME: - F2050
ANALYSED MODEL: - Long-legged Wading Bird FCI

>>> ALTERNATIVE SCENARIO
TIME INTERVAL: - 1975 (1 year)
HYDROLOGIC REGIME: - D13R
ANALYSED MODEL: - Long-legged Wading Bird FCI

REGIONAL SUBDIVISIONS: - ATLAS Subregions (poly)

This is not optimal control, but rather is a scenario analysis in which we compare and contrast the impacts of alternative management plans

But there are numerous uncertainties due to incomplete knowledge of system processes and species dynamics, stochasticity in model inputs (e.g. weather patterns, mortality, etc.), complex model structure, and inaccuracy in the measurement of parameters

To deal with this we use a relative assessment protocol

Fuller, M. M., L. J. Gross, S. M. Duke-Sylvester, and M. Palmer. 2008. Testing the robustness of management decisions to uncertainty: Everglades restoration scenarios. *Ecological Applications* 18:711-723.

Relative assessment

$i = 1, 2, \dots, k$ indicate a collection alternative scenarios, defined by a collection of anthropogenic and environmental factors that affect the modeled ecosystem or a particular model configuration.

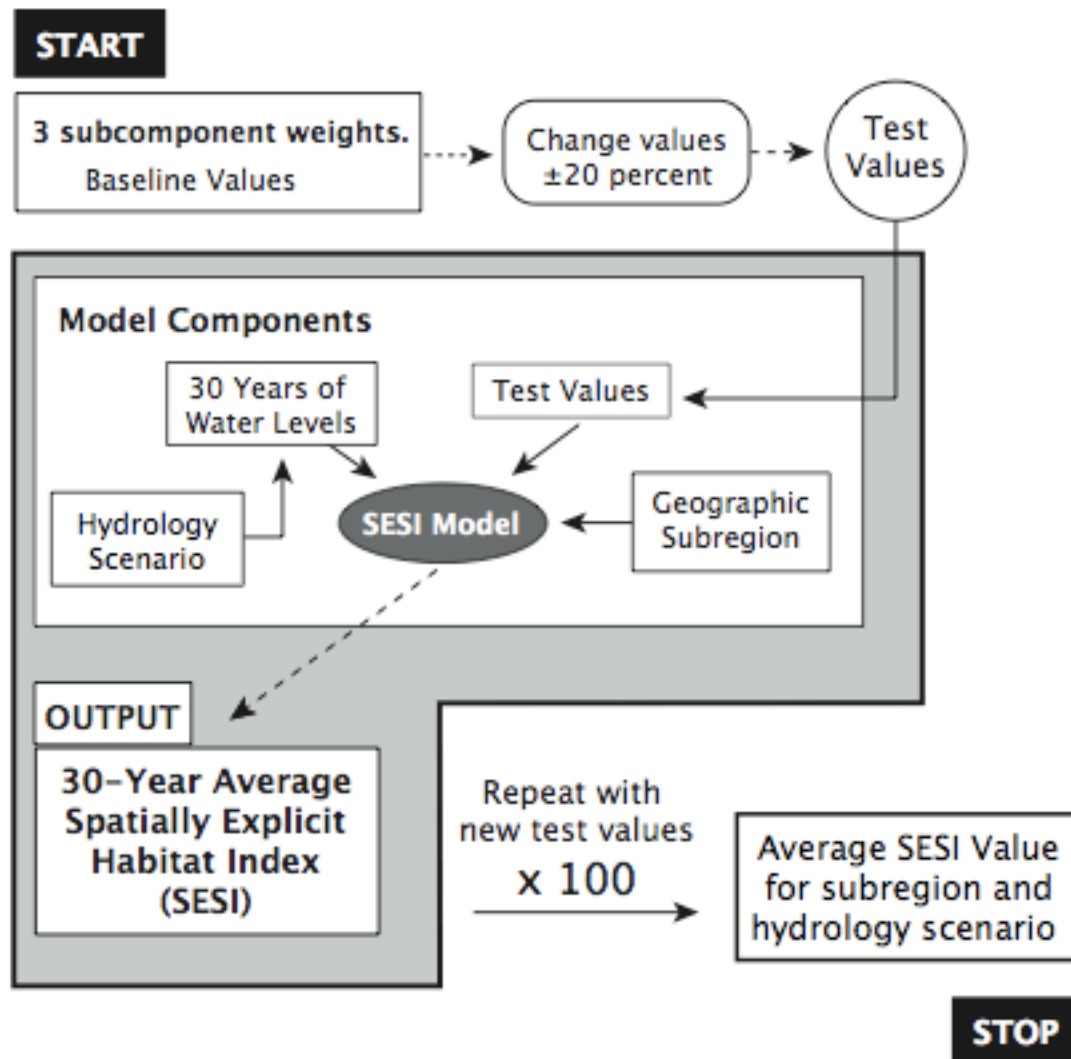
P represents a particular configuration of the model, including the values of model parameters, specific assumptions and functional forms used.

$E_j, j = 1, 2, \dots, n$ are anthropogenic and environmental factors (rainfall, fire events, etc.)

$M_i (P, E_1, \dots, E_n)$ for $i = 1, 2, \dots, k$ are the output of a model which projects the response of natural system components under scenario i with model parameters P and environmental inputs E_j .

$R (M_1 (P, E_1, \dots, E_n), \dots, M_k (P, E_1, \dots, E_n))$ is a ranking of the scenarios based upon evaluation criteria and utilizing the results of the models

A relative assessment is **robust** to a particular variation in model parameters and/or environmental inputs if the variation does not change the ranking R . When the model results M_i are recomputed based upon a particular variation in the E_j and P , the rank order of the models in R does not change.



- Repeat for each hydrology scenario (F2050 & D13R)
- Repeat for each subregion.

START

STEP

1 Compile 30 year water level base pattern:



2 Select the 5 wettest years from base pattern to form one block of 5 years:



3 Randomly reorder the 5 years selected in step 2:



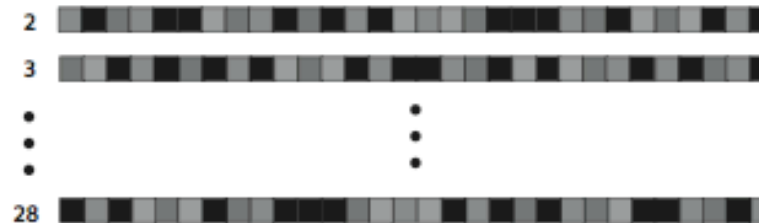
4 Repeat steps 2 and 3 five more times:



5 Combine the blocks created in steps 2 - 4 into a single 30-year sequence:



6 Repeat steps 2 - 5 27 more times to create a total of 28 30-year sequences:



7 Calculate a mean SESI value for each 30 year sequence, for each hydrologic plan, and a grand mean for each hydrologic plan:

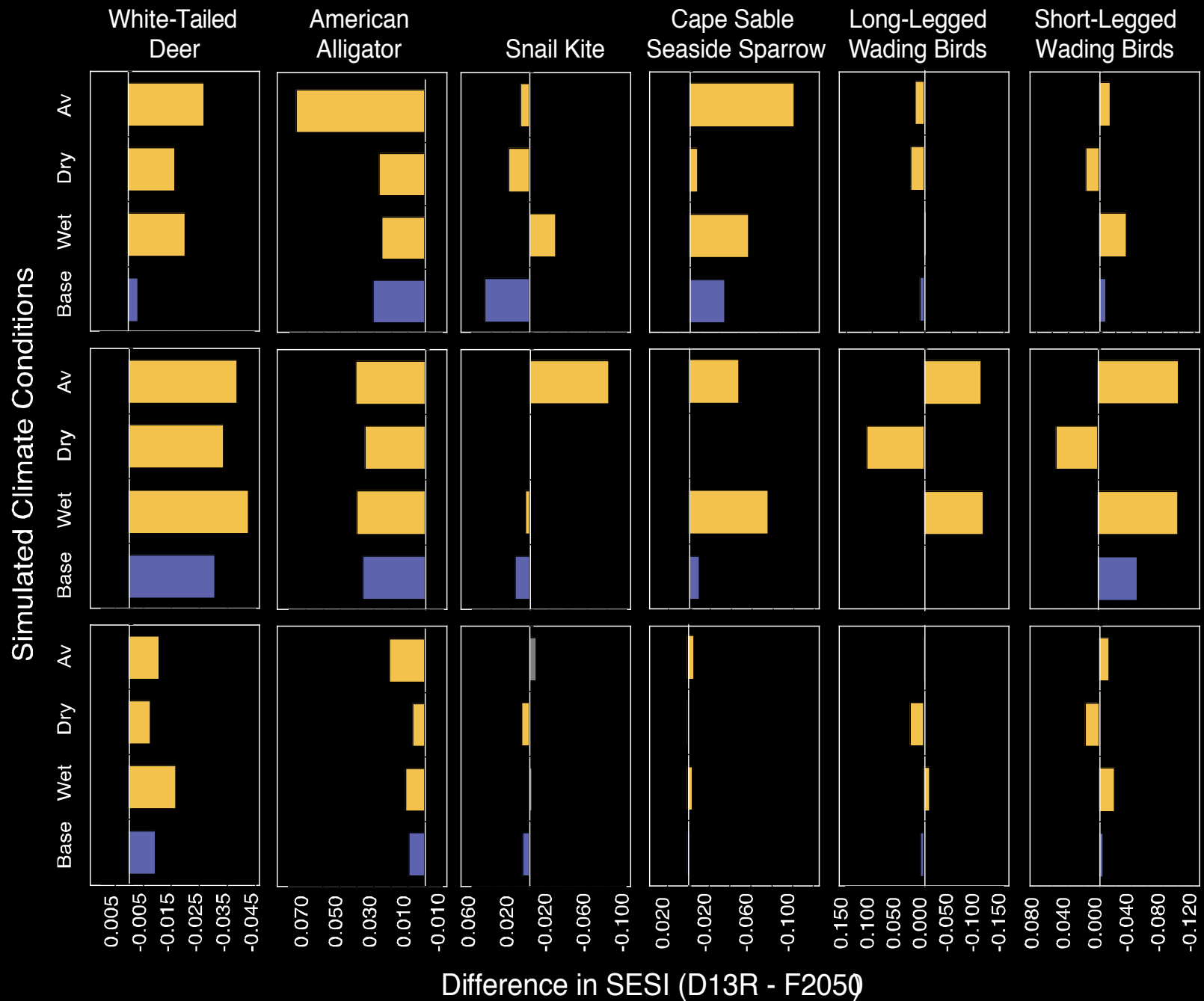
| Example Count | Hydrologic Plan | |
|------------------|------------------------|--------|
| | D13R | F2050 |
| | White-Tailed Deer SESI | |
| 1 | 0.1365 | 0.1535 |
| 2 | 0.1366 | 0.1533 |
| 3 | 0.1367 | 0.1534 |
| ⋮ | ⋮ | ⋮ |
| 28 | 0.1366 | 0.1535 |
| Grand Mean | 0.1366 | 0.1534 |

8 Calculate the difference in the grand means of the plans.

$$D = D13R - F2050 = -0.0168$$

STOP

Effect of Simulated Climate on Scenario Ranking



Lessons from ATLSS - Doing the Modeling:

- **Work closely with those with long experience in the system being modeled and use their experience to determine key species, guild and trophic functional groups on which to focus.**

Moderate the above based first on the availability of data to construct reasonable models, and secondly on the difficulty of constructing and calibrating the models.

Don't try to do it all at once - start small - but have a long-term plan for what you wish to include overall, given time and funding.

Lessons from ATLSS - Doing the Modeling:

Leave room for multiple approaches: don't limit your options.

In the face of limited or inappropriate data, use this as an opportunity to encourage further empirical investigations of key components of the system.

Build flexibility in as much as possible.

Be flexible about what counts as success.

Lessons from ATLSS - Personnel Matters:

- **Build a quality team who respect each others abilities and won't second guess each other, but who accept criticism in a collegial manner.**

Keep some part of the team out of the day-to-day political fray.

Be persistent, and have at least one member of the team who is totally dedicated to the project and willing to stake their future on it.

Do whatever you can to maintain continuity in the source of long-term support for the project.

Lessons from ATLSS - Interacting with Stakeholders:

- **Constantly communicate with stakeholders.**

Regularly explain the objectives of your modeling effort, as well as the limitations, to stakeholders. Be prepared to do this over and over for the same people, and do not get frustrated when they forget what you are doing and why.

Be prepared to regularly defend the scientific validity of your approach.

Lessons from ATLSS - Interacting with Stakeholders:

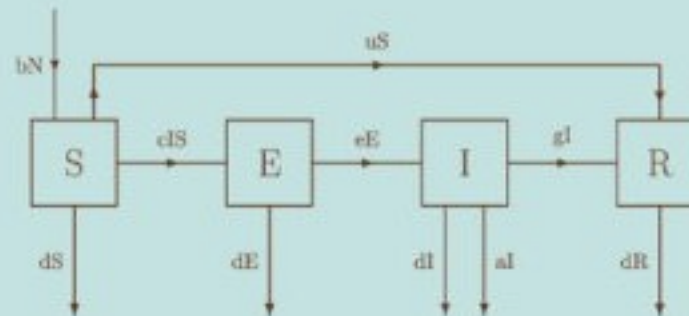
Don't limit your approach because one stakeholder/funding agency wants you to.

Be prepared for criticism based upon non-scientific criteria, including personal attacks.

Ignore any of the stakeholders at your peril.

Chapman & Hall/CRC
Mathematical and Computational Biology Series

Optimal Control Applied to Biological Models



Suzanne Lenhart
John T. Workman

 Chapman & Hall/CRC
Taylor & Francis Group



Optimal Control of Disease

Rabies in Ohio

Model

- Spatially explicit dynamics.
- Search for optimal strategy.

PARAMETERS

- * Cost of control efforts
- * Control Success Rate
- * Disease Dynamics

Data

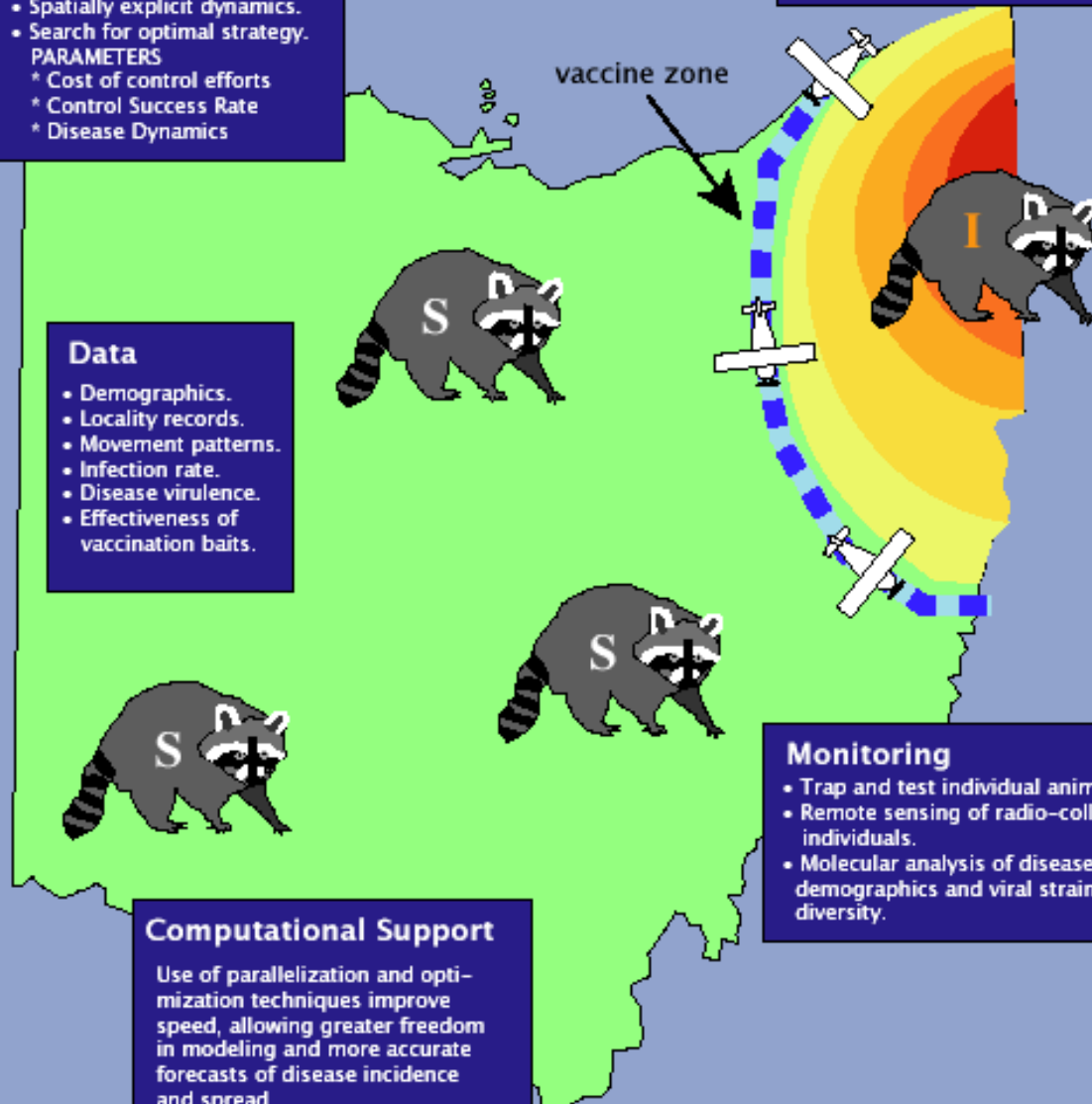
- Demographics.
- Locality records.
- Movement patterns.
- Infection rate.
- Disease virulence.
- Effectiveness of vaccination baits.

Computational Support

Use of parallelization and optimization techniques improve speed, allowing greater freedom in modeling and more accurate forecasts of disease incidence and spread.

Control Strategy

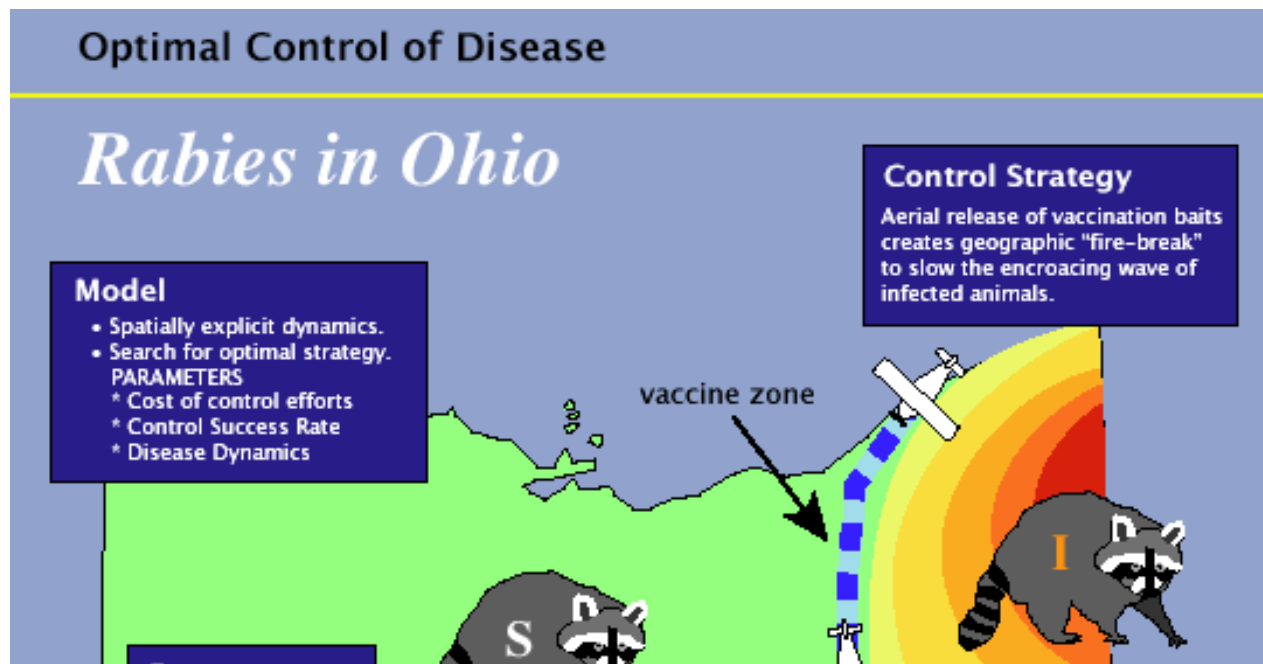
Aerial release of vaccination baits creates geographic "fire-break" to slow the encroaching wave of infected animals.



Monitoring

- Trap and test individual animals.
- Remote sensing of radio-collared individuals.
- Molecular analysis of disease demographics and viral strain diversity.



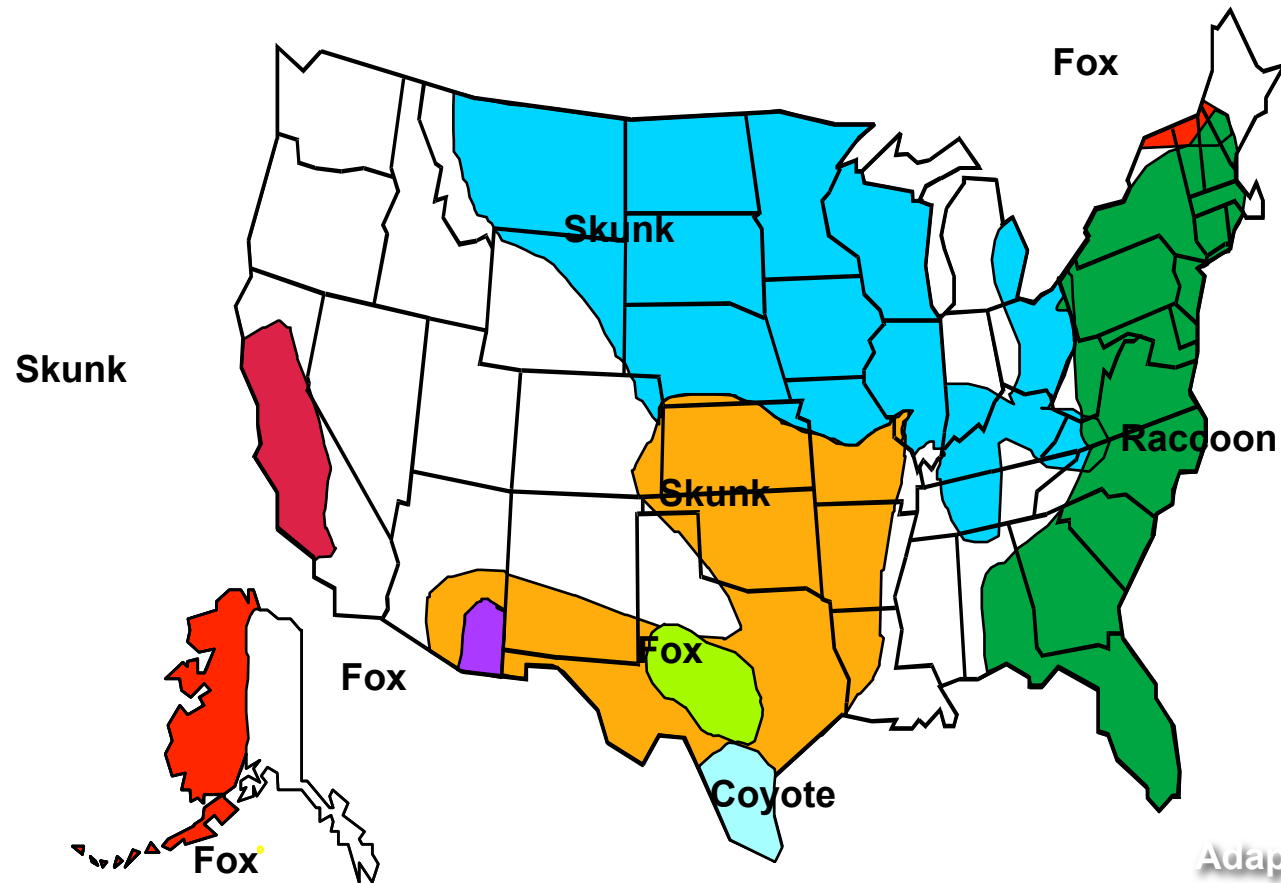


Ding, W., L. J. Gross, K. Langston, S. Lenhart and L. A. Real. 2007. Rabies in raccoons: optimal control for a discrete time model on a spatial grid. *Journal of Biological Dynamics* 1:379-393.

Asano, E., L. J. Gross, S. Lenhart and L. A. Real. 2008. Optimal control of vaccine distribution in a rabies metapopulation model. *Mathematical Biosciences and Engineering* 5:219-238.

Clayton, T. J., S. Duke-Sylvester, L. J. Gross, S. Lenhart, and L. A. Real. 2010. Optimal control of a rabies epidemic model with a birth pulse. *Journal of Biological Dynamics* 4:43-58

Distribution of rabies in terrestrial reservoirs



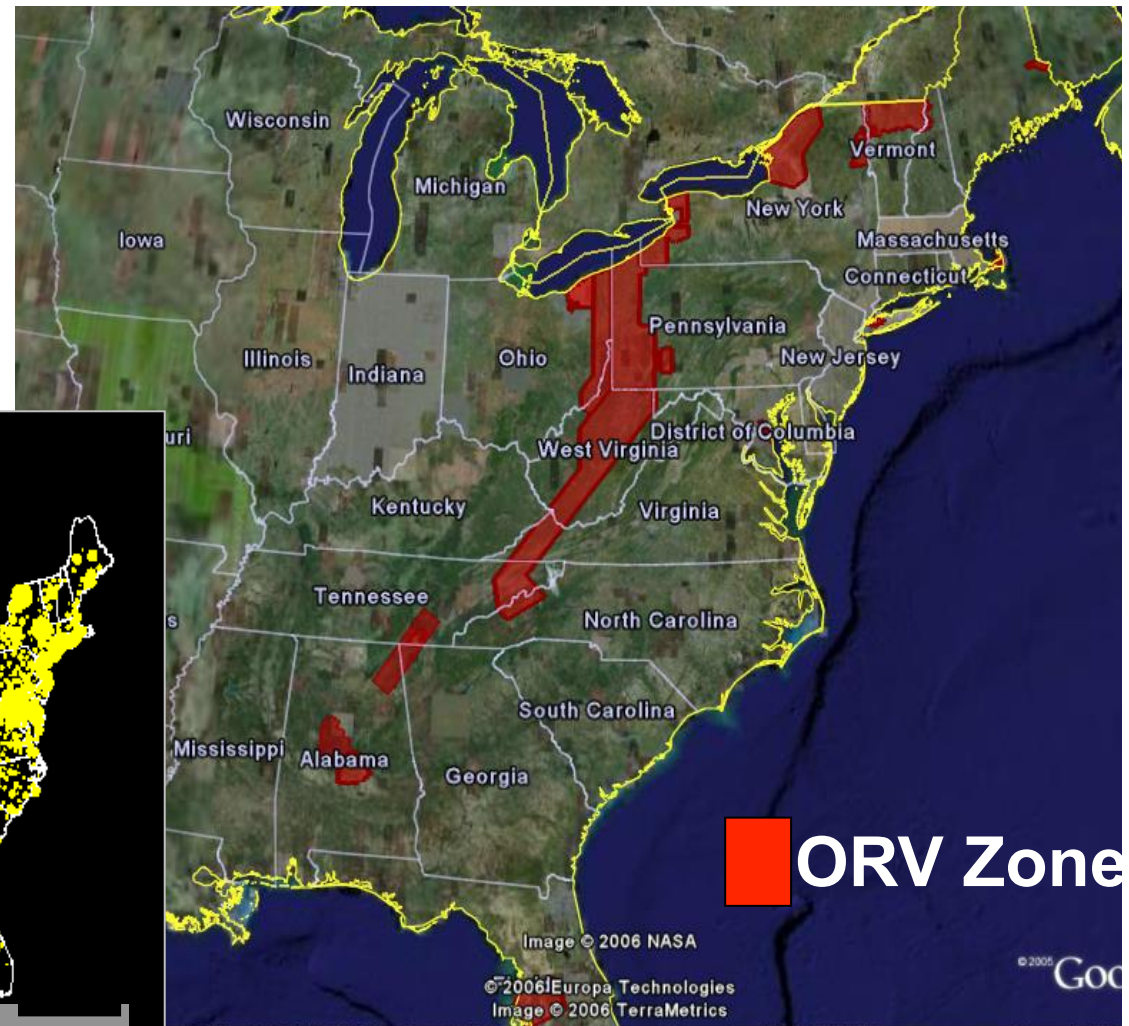
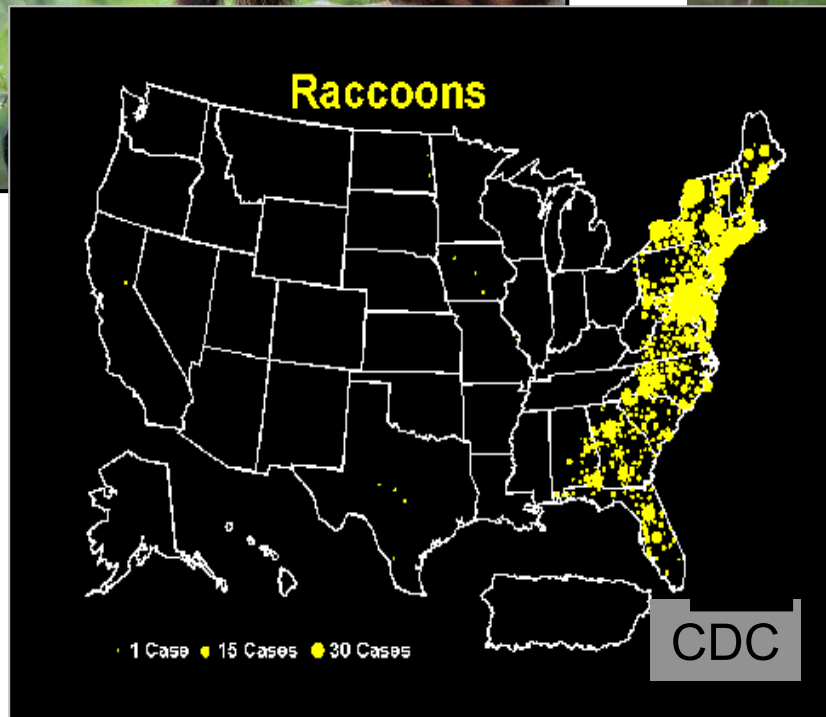
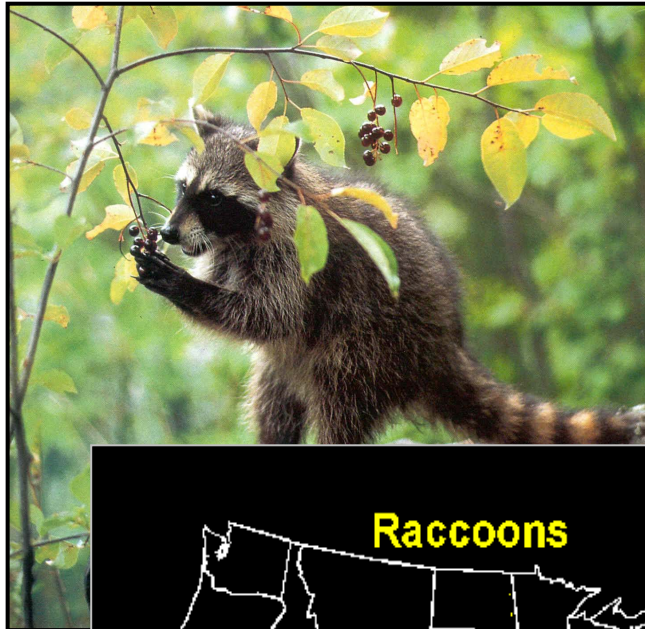
Adapted from
CDC



Prevent spread to new areas west and north of current distribution



Explore elimination strategies



Objectives for raccoon rabies models

- Account for dynamics of localized (individual and population) response to vaccination schedules as affected by seasonality
- Account for spatial aspects of disease spread including impacts of spatio-temporally-explicit vaccination patterns
- Provide methods to evaluate alternative management scenarios (e.g. vaccination, culling) as specified by stakeholders
- As potential comparators to simpler approaches, develop methods for determining the “best” management using criteria established by stakeholders, including economic ones

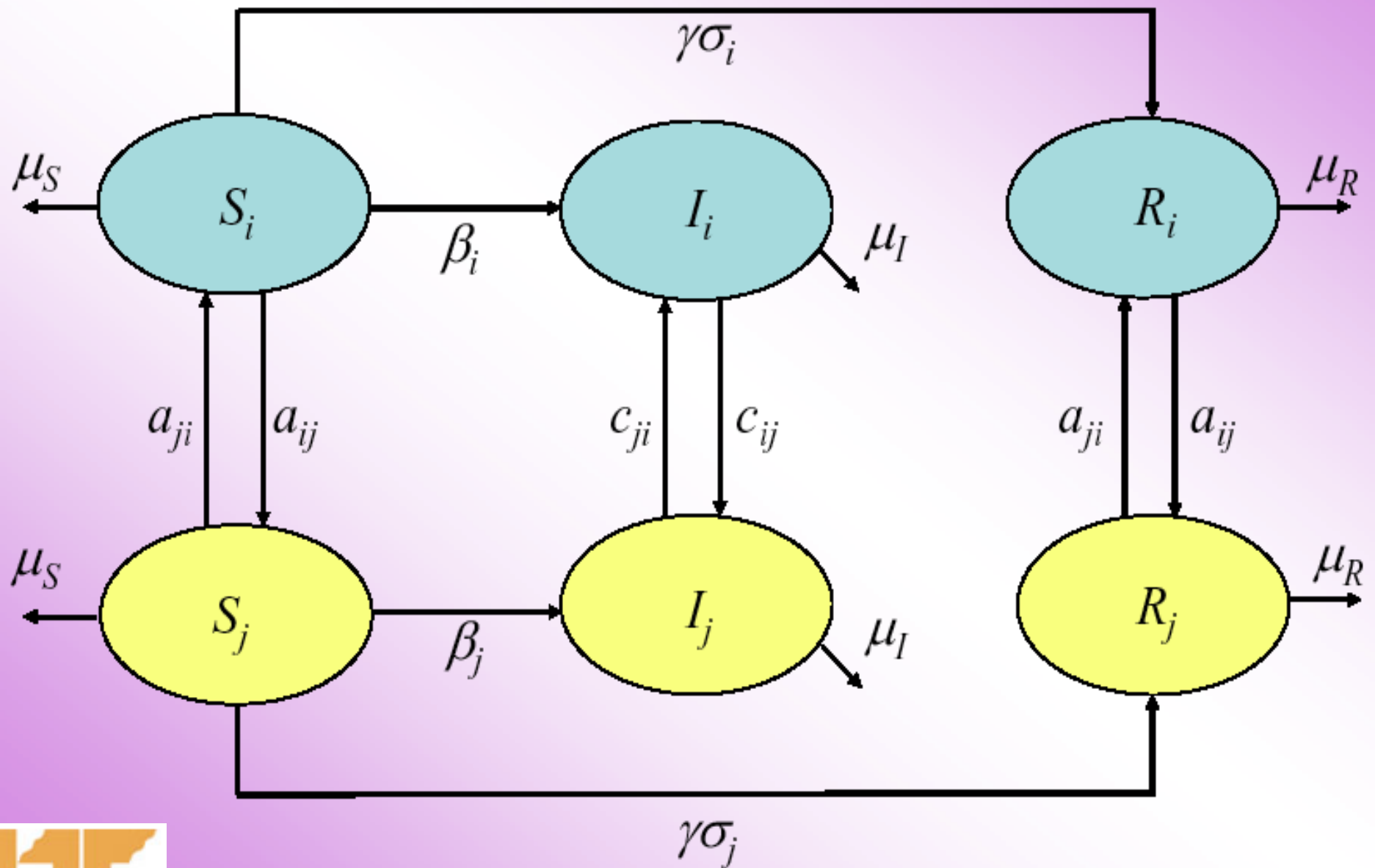


Objectives for raccoon rabies models

- Provide the capability to utilize spatial data readily available to management agencies
- Provide methods to evaluate trade-offs such as between expenditures for barriers and surveillance programs
- Provide methods to account for genetics of transmission and determination of interspecies transmission impacts
- Provide methods to account for impacts of population structure (age) on spatial spread
- Provide methods to carry out risk assessments for management actions at various spatial scales, considering impacts of multiple species and spatial and temporal variation in habitat conditions (including climate change impacts)



Flow between spatial region i and region j



$$S(t) = (S_1(t), S_2(t), \dots, S_n(t))$$

where $S_i(t)$ is the number of susceptibles in subpopulation i .

$$I(t) = (I_1(t), I_2(t), \dots, I_n(t))$$

where $I_i(t)$ is the number of infecteds in subpopulation i .

$$R(t) = (R_1(t), R_2(t), \dots, R_n(t))$$

where $R_i(t)$ is the number of individuals immune to the disease in subpopulation i .

$$\mu(t) = (\mu_S, \mu_I, \mu_R)$$

$\mu(t)$ is the mortality rate in each class: S , I and R .

$$\beta(t) = (\beta_1, \beta_2, \dots, \beta_n)$$

$\beta_i(t)$ is the rate of transmission in subpopulation i .

$$\sigma(t) = (\sigma_1(t), \sigma_2(t), \dots, \sigma_n(t))$$

$\sigma_i(t)$ is the rate of removal(control) of susceptibles from subpopulation i to the immunes due to vaccinations.

γ is the efficacy of vaccination.

$A(t) = (n \times n)$ matrix

where the matrix element a_{ij} is the rate of transition of non-infecteds(susceptible and immune classes) from subpopulation i to subpopulation j .

$C(t) = (n \times n)$ matrix where the matrix element c_{ij} is the rate of transition of infecteds from subpopulation i to subpopulation j .



Base model - with no growth (births)

$$(1) \quad \frac{dS_i}{dt} = -\beta_i S_i I_i - \gamma \sigma_i S_i + \sum_{j, j \neq i}^n a_{ji} S_j - \sum_{j, j \neq i}^n a_{ij} S_i - \mu_S S_i$$

$$(2) \quad \frac{dI_i}{dt} = \beta_i S_i I_i + \sum_{j, j \neq i}^n c_{ji} I_j - \sum_{j, j \neq i}^n c_{ij} I_i - \mu_I I_i$$

$$(3) \quad \frac{dR_i}{dt} = \gamma \sigma_i S_i + \sum_{j, j \neq i}^n a_{ji} R_j - \sum_{j, j \neq i}^n a_{ij} R_i - \mu_R R_i$$

ICs :

$$(4) \quad S_i(0) = S_{i0}, \quad I_i(0) = I_{i0}, \quad R_i(0) = R_{i0}$$

Control(Vaccination) :

$$(5) \quad 0 \leq \sigma_i \leq \sigma_{\max} \quad \text{for } i = 1, 2, \dots, n.$$

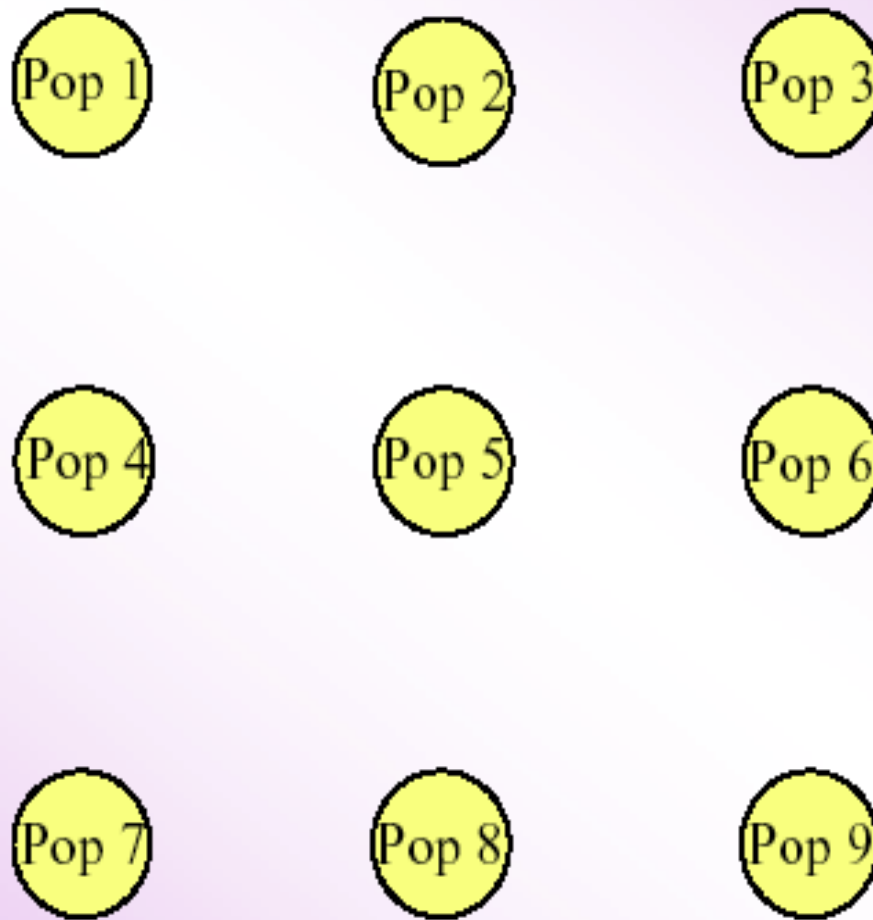
We wish to minimize J = the total number of infecteds and the cost associated with vaccination

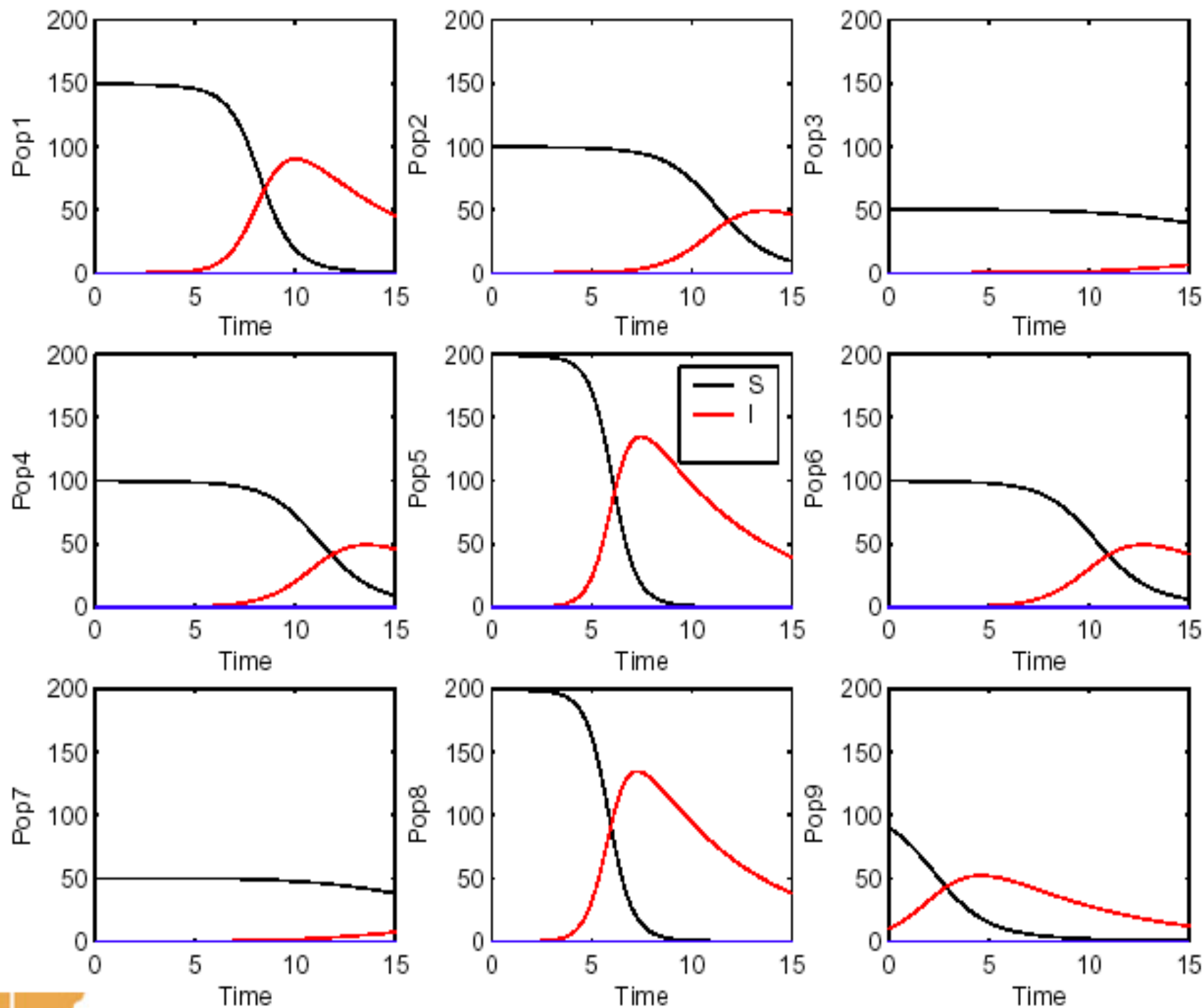
$$J(\sigma) = \sum_{i=1}^n \int_0^T I_i + \frac{\alpha}{2} \sigma_i^2 dt$$

To solve, use Pontryagin to develop adjoint equations, make an initial guess for the control, use a forward sweep of the model SIR equations, a backward sweep of the adjoint equations (these have final-time conditions at T), update the controls, and iterate until a stopping condition is met.



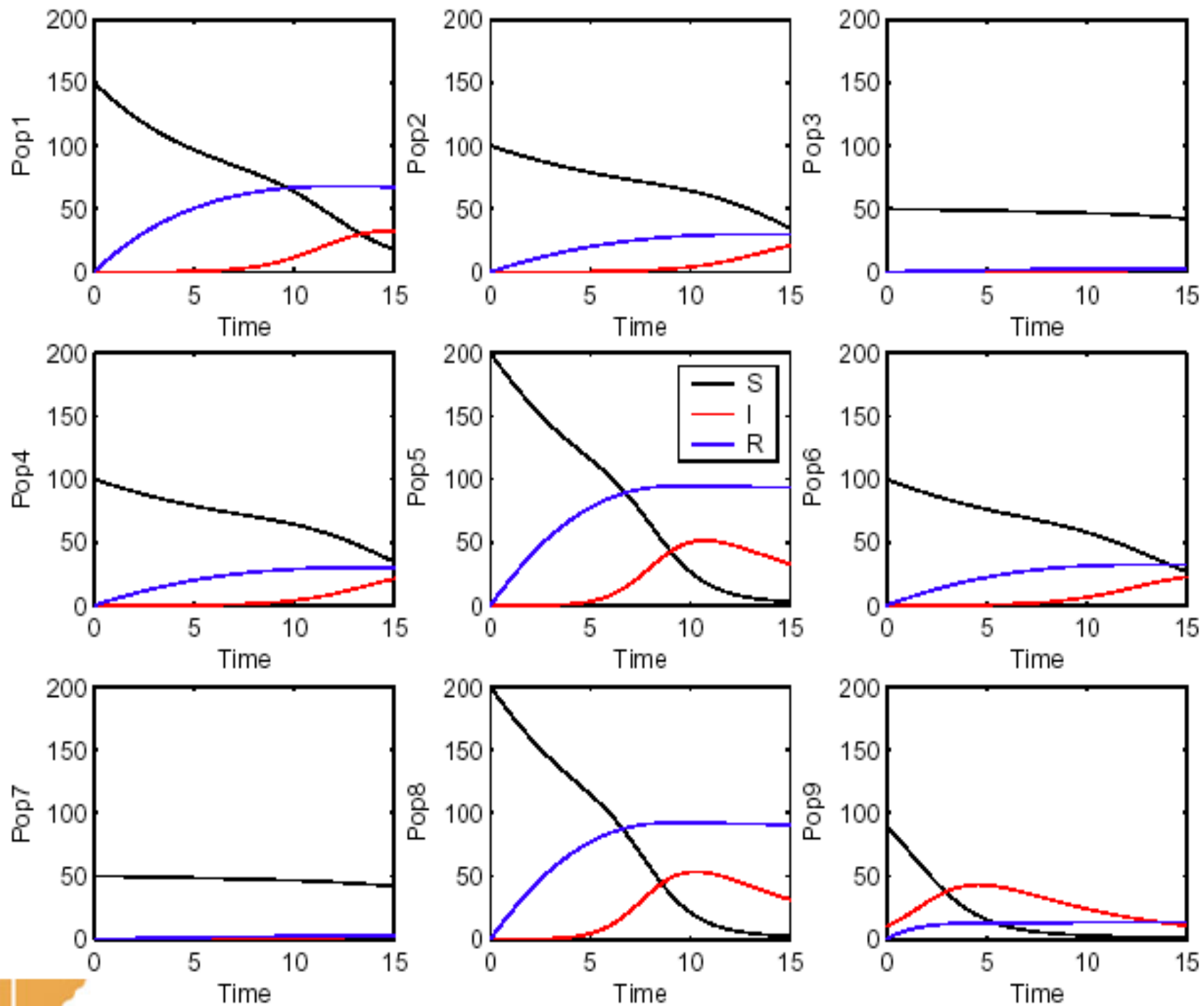
Example spatial layout with $n = 9$. An example will introduce infectives into Pop 9, will have different initial susceptible populations in different locations, and compare spread without vaccination to that with optimal vaccination





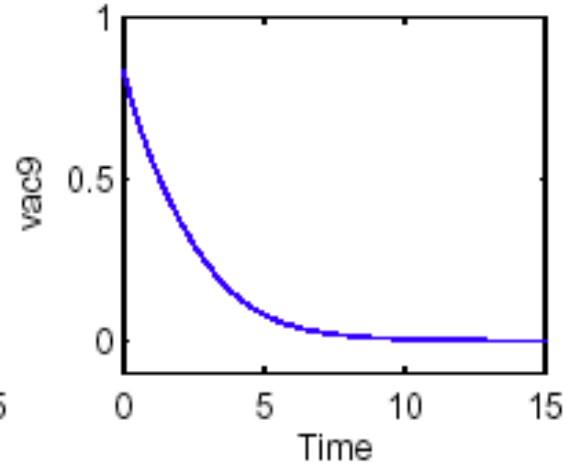
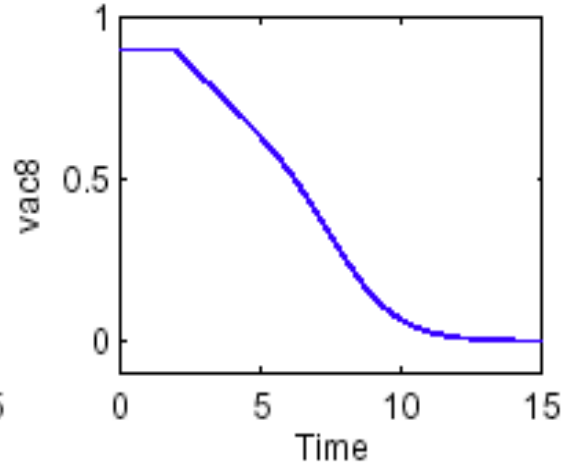
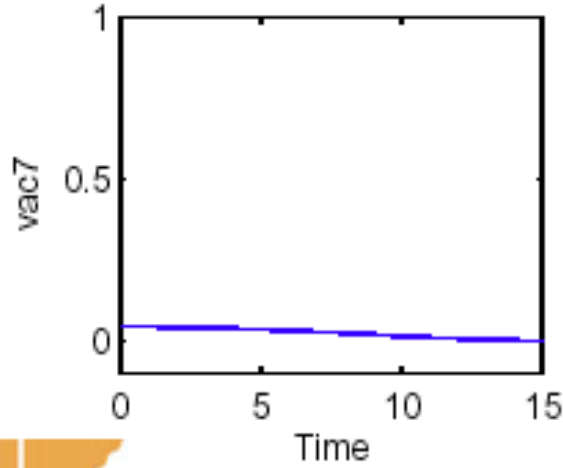
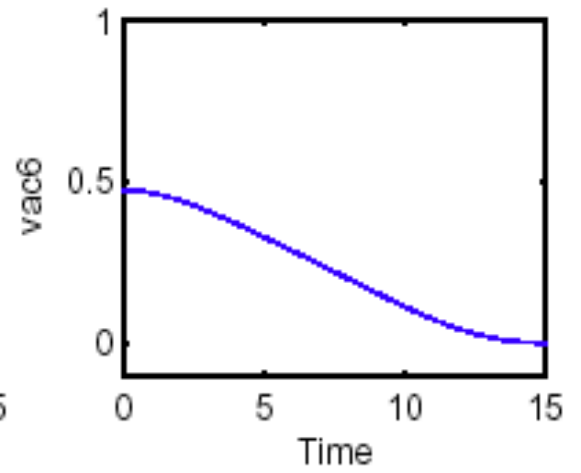
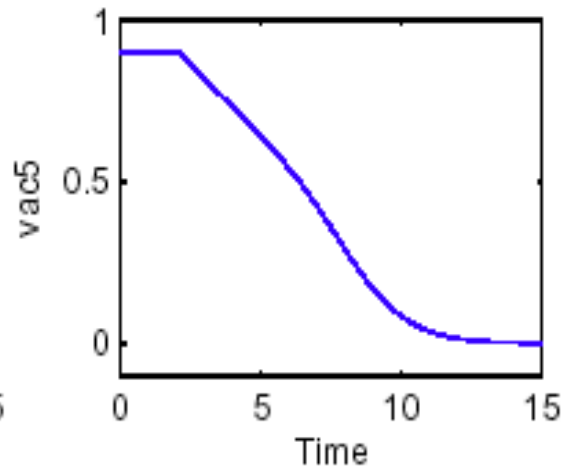
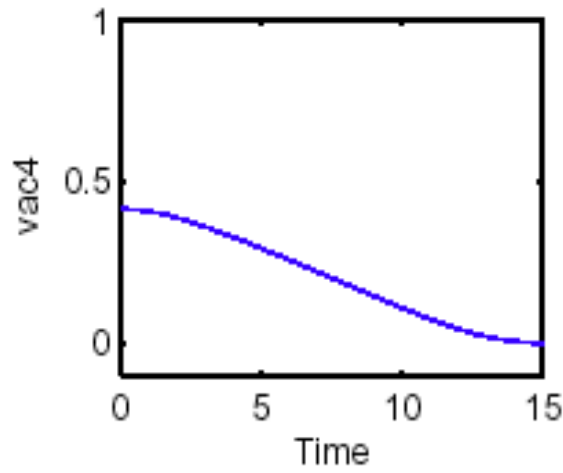
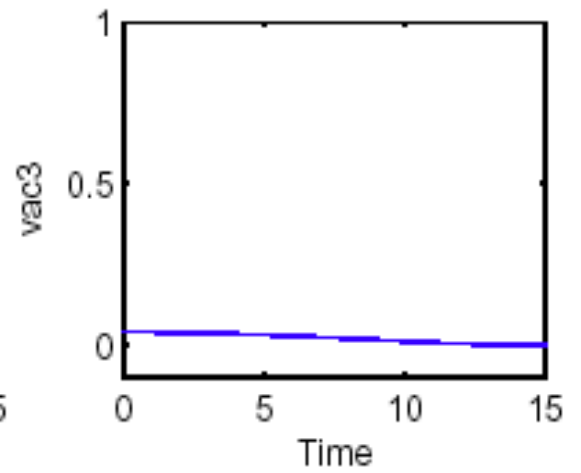
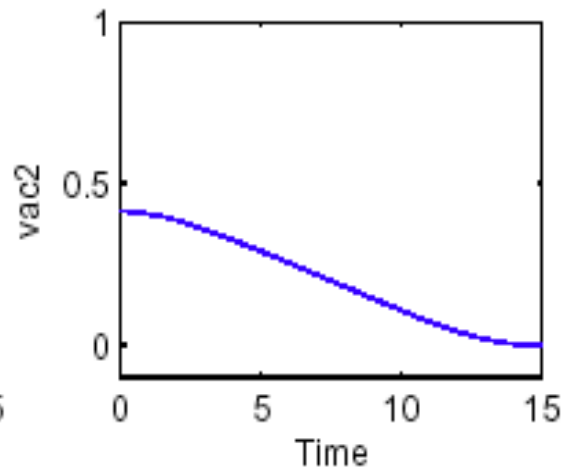
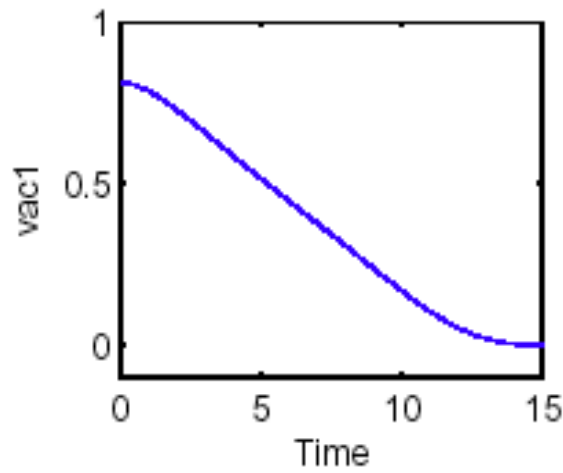
No vaccination





Optimal vaccination

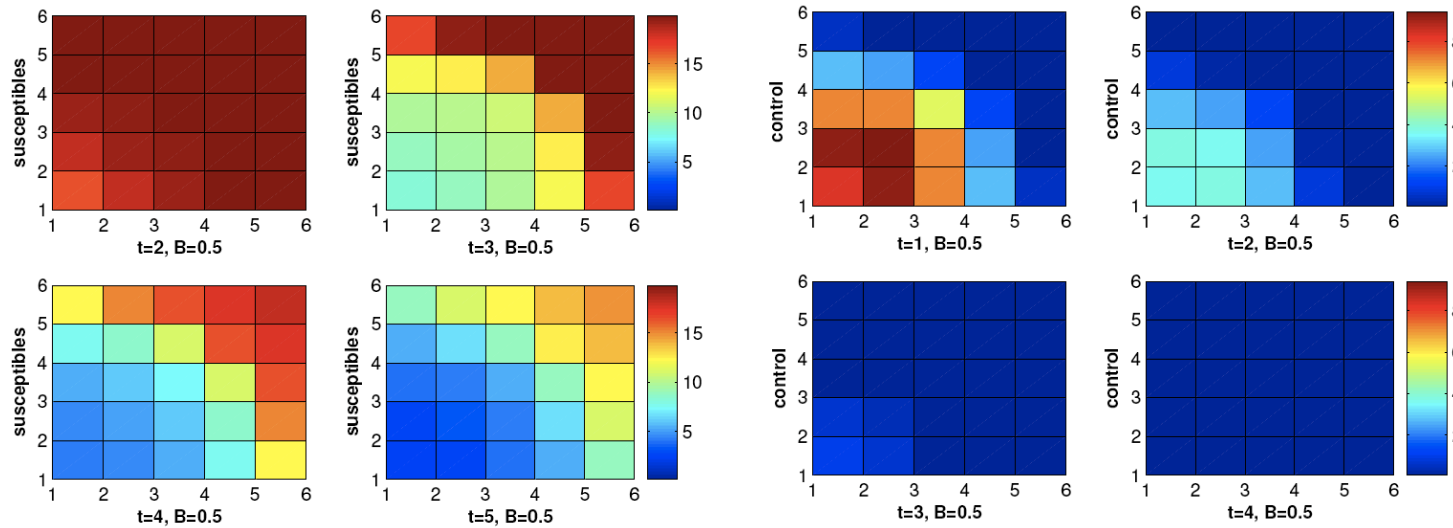




Optimal spatial vaccination strategy

Other optimal control rabies models we've done have:

- Developed discrete-time control on a spatial grid



- Included an exposed class
- Included dynamics of the baits
- Included limits on amount of vaccine available
- Included seasonal birth-pulses leading to a hybrid, discrete-linked-to-continuous model