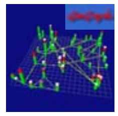

Rigorous Inference with Spatial Agent-Based Computational Laboratories

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University of Maryland
21 March 2006

Office of Naval Research

MIDAS

Outline – Inference with Agent-Based Comp Labs

- **W**ho we Are – Funding, Lab Team, GeoGraph Comp Lab
- **I**ntro – Relevance and Importance of Pandemic Questions
- **M**ethods – GeoGraph Pandemic Model, Tools, Experiments
- **R**esults – Preliminary Rankings of High-Risk US Cities
- **A**nalysis – *How much can we trust our results?*
- **D**iscussion – Limitations, Further Work, and Relevance

Research Funding and Projects

Office of Naval Research

- Office of Naval Research (ONR)
  - The GeoGraph 3D Simulation Platform
  - Models of Epidemics and Civil Violence
  - Optimization of Crisis Interventions

MIDAS

- National Institutes of Health (NIH)
  - NIGMS – Models of Infectious Disease Agents Study (MIDAS) (with JHU, Imperial College, Brookings)
  - **NVPO – Controlling Pandemic Influenza**
- Environmental Protection Agency (EPA)
  - Mid-Atlantic Regional Simulation
- Maryland Population Research Center (MPRC)
  - Life-cycle Dynamics in GeoGraph Agents

Computational Laboratories Lab Team


Steve

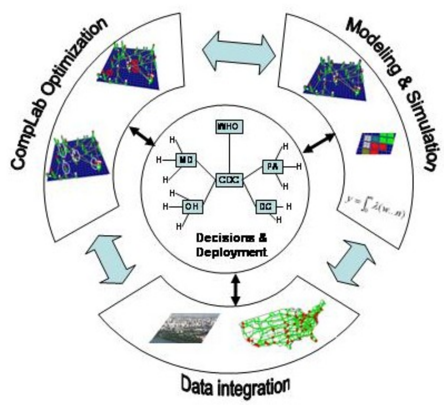

Ritvik


Chaoqing

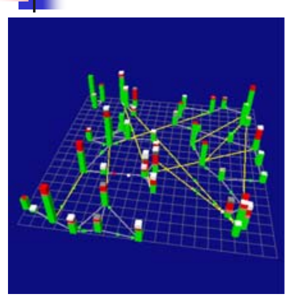

Jill


Alex

- **Steve Wendel**
  - Research Manager and Lead Programmer
- **Ritvik Sahajpal**
  - Computer Science, Analytical Measures
- **Chaoqing Yu**, PhD
  - Concept Maps and Expert Rule Systems
- **Tim Heleniak**
  - Demographics and Regional Modeling
- **Alex Torrella**
  - Undergraduate Assistant
- **Jill Bigley Dunham** (George Mason)
  - Computer Science, Mathematics, Networks
- **Robert Najlis** (NYC)
  - Consulting Agent-Based Programmer



The GeoGraph 3D Agent-Based Computational Laboratory (Univ of Maryland)

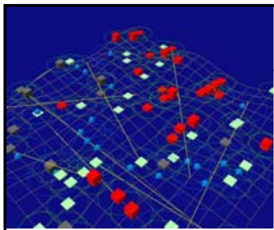


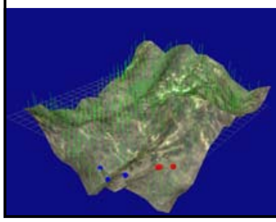
http://jasss.soc.surrey.ac.uk/7/1/7.html

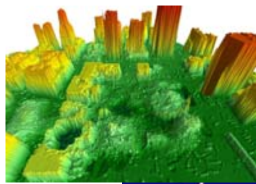
A general purpose computational laboratory for modeling *& inference*:

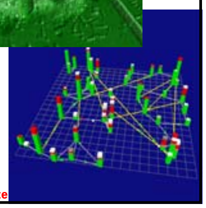
- heterogeneous mobile agents
- on richly-structured network/terrain landscapes
- at all scales from buildings to global networks of cities
- either synthetic landscapes or real-world GIS / RS landscapes
- network and/or 3D terrain

Multi-Scale Synthetic and Remote Sensing GeoGraph Simulation Landscapes









Agent-Based Models

- *Agent* is a generic term for any constituent entity whose behavior we wish to model, and for its representation within the model.
- For example, an agent may be, or may represent, a plant, an animal, or a person.
- Note! Even a group such as a family, a country, or a corporation may be regarded as a behavioral agent for purposes of understanding a given system, depending upon the model's scale and degree of generalization.
- Agent-based models are also called individual-based models, especially in ecology. But we mean the term to be more general than a 1:1 mapping of individuals.

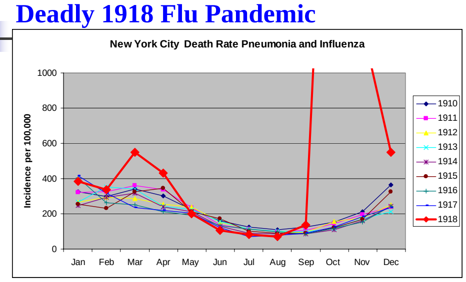
Computational Laboratories

To paraphrase Lance Armstrong:
It's not about the model.

We define a computational laboratory as a well-specified agent-based simulation model coupled with complementary tools for search and optimization, statistical analysis, and structural measures such as network analysis.

Computational laboratory practices include calibration, validation when possible, careful experimental design, and thorough testing, sensitivity analysis, risk analysis and, above all, the art of scientific investigation, a sense of evidence, and sufficient replications for strong inference.

Deadly 1918 Flu Pandemic



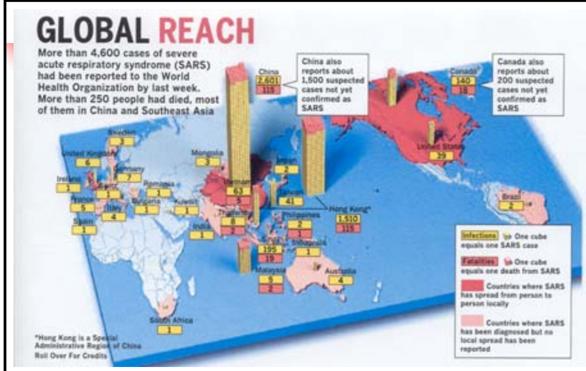
- **Killed 30 to 100 million people**
- **Out of a world population only ~ 1.7 billion**
- **Most deaths within a span of only 16 weeks**
- **From mid-September to mid-December 1918**

Incipient H5N1 Influenza Pandemic

- H5N1 Avian Influenza
- Human case-mortality rate ~55% (96/175 lab confirmed)
- Spreading rapidly worldwide via migrating birds.
- Not yet spreading easily human-to-human
- How best to prepare, in case it does?
- Limited Resources and Difficult Interventions
  - antiviral drugs, vaccines, National Guard troops, etc.
  - closing schools or work, travel restrictions, quarantine
- How to make the best use of interventions?
- **Harness geographic structure to amplify the protective leverage of available resources.**

Macroeconomic Consequences of Pandemic Influenza (Feb 2006) Lowy Institute for International Policy

- Mild Scenario – similar to 1968-1969 Hong Kong Flu
  - 1.4 million deaths
  - GDP loss of 0.8% (~$US 330 Billion)
- Medium Scenario – similar to the 1957 Asian Flu
- Severe Scenario – similar to the 1918-1919 Spanish Flu
- Ultra Scenario – worse than the 1918 Flu
  - 142.2 million deaths
  - GDP loss of ~$4.4 Trillion



(Map by Joe Lertola, *TIME* Magazine 5 May 2003, Data as of 25 April 2003)

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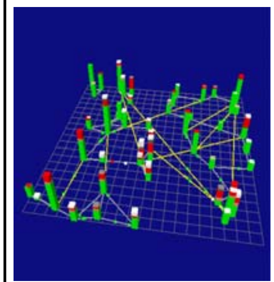
GeoGraph Pandemic Model



- Colored bars are city populations
- People travel between cities, spreading the disease (SEIR meta-population)
- Bar charts show health status:
  - Green – susceptible
  - Pink – infected
  - Red – infectious
  - White – immune (naturally or artificially)
  - Gray – dead
- Links are roads and/or airline routes
- R_0 may be modified by:
  - individual characteristics
  - super-spreader events/circumstances
  - seasonality (sine wave)

(Dibble and Feldman (2004) http://jasss.soc.surrey.ac.uk/7/1/7.html)

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Key Research & Policy Questions

- **Which cities are at greatest risk (no intervention)?**
  - **when locations of initial (US) cases are not yet known?**
  - **when location(s) of initial cases are known.**
- What are the best possible geographic (and possibly also temporal) deployments of limited resources or high-cost interventions?
  - How best to use geographic structure to leverage effectiveness?
- Which airline flights, train routes, or highways should be monitored, quarantined, or blocked?

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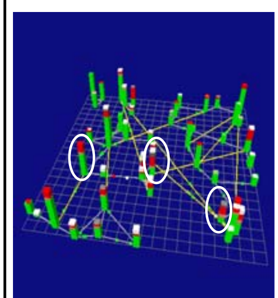
1. Identify High-Risk Cities



- Run 4,700 simulations
- Each with its own random history and initial conditions
- Which cities are consistently at higher risk for levels of exposure than other cities?

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Optimizing Interventions for Controlling Epidemics

Genetic Algorithm

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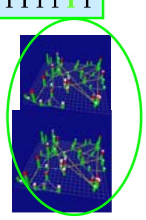
Intervention: types of control measures and geographic deployment of resources for each.



- Run many GeoGraph simulations ("epidemic histories") to evaluate each intervention.

1. A Genetic Algorithm (GA) evolves highly effective interventions, *based on simulation results.*
2. GA then assists with risk analysis by seeking best-case and worst-case (Murphy's Law) outcomes for each of the best interventions.

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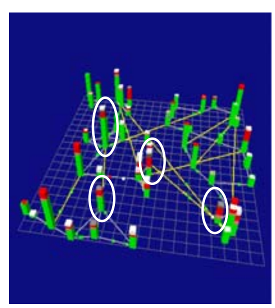
2. City Interventions



- Select specific cities to receive additional resources to control the epidemic.
- Run the simulation many times to evaluate each intervention.
- **Genetic Algorithm optimizes interventions.**

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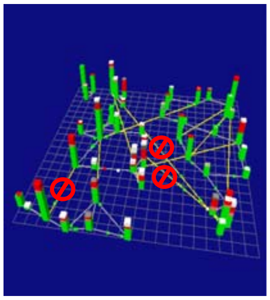
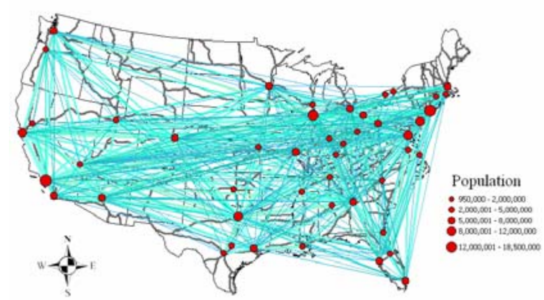
3. Transportation Interventions



- Select specific transportation links (e.g. airline flights) to monitor or to block.
- Run the simulation many times to evaluate each intervention.
- Genetic Algorithm optimizes interventions.

US 47-Cities Airline Network (100,000 passengers/link/year)



Calibrating Gravity Travel Behavior

- Trip Probability => whether to travel at all
  - Calibrated per Origin City via Empirical Data (trips / metro population)
- Destination Choice => where to go
  - Destination Probability ~ DestCityPopulation^0.9 * PathDistance^0.5
  - Parameters Calibrated per City via Empirical Data
  - Note: Distance parameter generally > 0! Not = -2. Because of overhead...
- **Need Data for Calibrating Other Travel Behavior (True O/D)**
  - **US Surface (Highways, Trains)**
  - **Global Air and Surface**
  - **Suggestions and data very much welcome!**

US Simulations for Relative Risks

- 4,700 Simulations of 100,000 Agents Each
  - 47 Largest US Metropolitan Areas
    - Combine SJC>SFO, ONT>LAX, BWI>WAS
  - 100 epiSeed random number seeds per city
- 3,156 Pandemics with Morbidity > 700
  - Define Risk as # of Infected Arrivals per City
  - Regressions to Explain Risk per City
    - When US origin city is unknown.
    - When US origin city is known.

Relative Pandemic Risks of Key US Cities

Initial City: Unknown	Initial City: A	Initial City: B	Initial City: E	Initial City: G
A	A	B	E	A
B	B	A	B	G
C	C	E	A	B
D	D	D	C	C
E	E	C	D	D
F	F	F	G	E
G	G	G	F	F
H	J	I	H	H
I	K	M	I	M
J	L	H	J	N

Generalizing Results to New Landscapes

Benchmark Regression on Node Risk
(as # Infected Arrivals)

	Estimate	Std. Err	Tvalue	Beta	Pr(>|t|)
(Intercept)	-34.545	3.694	-9.35	(NA)	6.3e-12 ***
mCPL_D	-0.019	0.006	-3.31	-0.187	0.0019 **
Degree	0.060	0.018	3.31	0.264	0.0019 **
log(empiricalPop)	2.513	0.267	9.43	0.727	5.0e-12 ***

Signif. codes: '***' 0.001 '**' 0.01 '*' 0.05

R-Squared: 0.881 Adjusted R-squared: 0.873

We can capture 87% of the variation in risk between cities with a parsimonious model, where our network measures provide additional and significant (at 99%) explanatory power over city population alone.

Thought Experiments

- Why bother with agent-based simulations?
  - Distributed, dynamic, heterogeneous, quirky behavior, spatio-temporally sensitive feedbacks.
- Are we really learning anything *new*?
  - E.g., does travel behavior determine risk? (no)
- How much does it matter if our parameters are wrong?
  - What if H5N1 turns out to be very different? (14-days?)
  - What if people panic or respond in weird ways?
- **When lives are at stake, what are the tradeoffs between undue haste and undue caution with modeling, inference, action?**

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Calibration and Validation

- **Epidemiology parameters**: MIDAS, Flu Experts, Data
  - incubation, latency, infectious duration, detection, mobility
  - mean, min, max, and variance of R_0s (idealized 1° cases)
- **Interventions**: Marty Cetron, CDC, other MIDAS models
  - Marty & Ben: intervention priorities and available resources
  - Other MIDAS models: effects of interventions on urban R_0s
- **Gravity vs Travel Data**: Seats/Link, Passengers/Trip
  - calibrate travel probability
  - test/validate gravity model vs travel data
  - hybrid model? empirical travel network, gravity patterns?

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Calibrating for Inference

- For ordinary academic research, we choose our # rewinds to ensure significance of our results. I.e. we purposefully “waste” CPU cycles.
- For a pandemic emergency, we want high confidence, BUT we also want to explore interventions, scenarios, and risk as thoroughly as possible.
- So we do well to establish the following returns to:
  - # of cities: are more always better, to learn key lessons?
  - # of agents: for each # cities, how many agents overall?
  - # of runs: to differentiate outcomes among allocations for each GA string
  - # of runs: to fully explore risk or degree of uncertainty
  - AND are these the same across scenarios & interventions?

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Tradeoffs re Calibrating for Inference

- For ordinary academic research, we choose our # replications (# obs) to ensure significance of our results. I.e. we purposefully “waste” CPU cycles.
- **For a pandemic emergency, we want high confidence, BUT we also want to explore interventions, scenarios, and risk as thoroughly as possible.**
- So we do well to establish the following returns to:
  - # of cities: are more always better, to learn key lessons?
  - # of links: does it matter whether we include all links? (10/yr?)
  - # of agents: for each # cities, how many agents overall?
  - # of runs: to differentiate outcomes among allocations for each GA string
  - # of runs: to fully explore risk or degree of uncertainty
  - AND are these the same across scenarios & interventions?

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Risk Analysis, in Depth

Evaluate key interventions for resilience wrt unexpected events. For each of the best geographic allocations for selected combination of intervention(s) and scenario(s):

- establish moments for outcomes (min, max, mean, and st dev) by *running* 1,000s to 10,000s of replications for each of the best geographic allocations, and
- use the meta-GA by *searching across* 10,000s to 1,000,000s of replication for the worst outcomes of our best alternatives. (Murphy’s Law analysis…)

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Optimization, in Depth

- For each selected combination of intervention(s) and scenario(s),
- use the meta-GA by running many (~10s to 100s) rewinds for each GA string,
- to evaluate outcomes for each geographic allocation of resources based on some f(moments) where moments are min, max, mean, st dev), and
- **the meta-GA evolves a set of the most effective geographic allocations.**

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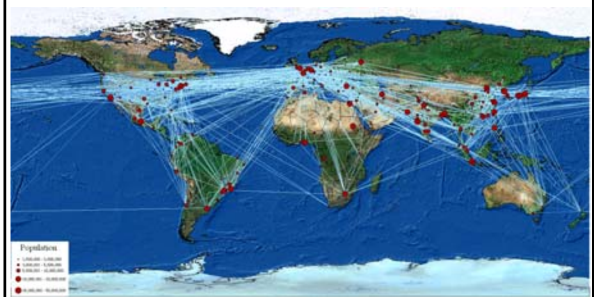
Limitations, Further Work, Relevance

- Limitations and Further Work
  - Sensitivity/Stability with respect to
    - # Agents, # Nodes, # Links, Travel & Epi Parms, Travel Modes
  - Business-as-Usual versus Pandemic Behavior (e.g. panic)
- *Complements* MIDAS Community Models
  - Focus attention on high-risk / high-benefit cities
  - City-specific results about effects of city interventions
- Effective Allocation of Limited Resources
  - Save as many lives as possible / slow pandemic as much as possible by taking advantage of network structure.
  - **Generalized measures supports rapid response for new landscapes without having to rerun simulations.**

Global Cities – Largest/Agglomerated 250



Thank you!

Thoughts, Questions, Suggestions?

Genetic Algorithms 101

Genetic Algorithms are set up by:

1. representing a problem solution as a string of parameters
2. defining a rule to determine the fitness of any given solution string
3. generating an initial population of strings

Subsequent generations are derived from previous generations by:

selection of strings for reproduction, with probability proportional to the relative fitness of each string

crossover between parent strings to recombine promising sets of parameters

mutation of the occasional parameter to encourage continued variety

Representing Problem Solutions as Strings

- Each chromosome is a string, where the "genes" are substrings that represent parameters (e.g. interventions)
- Representation decisions are at 2 levels:
  - How do you represent each parameter?
    - binary, Gray Code, decimal, alpha, other
    - generally, you want the smallest possible alphabet for each bit, which is why 0/1 is optimal if you can do that
  - **Fine ART: How do you arrange the parameters on the string?**
    - building block hypothesis – you want crossover to keep complementary parameters or "good ideas" together
    - you also want highly fit parents to be especially likely to produce highly fit children, this won't happen if too many of the potential recombinations are lethal (illegal or highly unfit solutions)

Genetic Algorithm Crossover & Mutation

Parent 1	A1	A2	A3	A4	A5	A6	A7	A8	A9
Parent 2	B1	B2	B3	B4	B5	B6	B7	B8	B9
Child 1	A1	A2	A3	B4	B5	B6	B7	B8	B9
Child 2	B1	B2	B3	A4	A5	A6	C7	A8	A9

Generating an Initial Population of Strings

- This initial population represents your first generation in the GA.
- It is almost always completely random.
- I.e., you want each chromosome to be a correct representation for a solution to your problem, but beyond that you can generate its parameters completely randomly.
- It is as though you put all the valid parameter values for each gene into a hat, then draw them out randomly (with replacement) to fill in the appropriate genes on each string.
- Do this until you have as many strings as you need for your first generation.

Running the Genetic Algorithm

- Subsequent generations are derived from previous generations by:
  - **selection** of strings for reproduction (proportional to fitness)
  - **crossover** between strings (to mix and match good ideas)
  - **mutation** of the occasional parameter (but not too often!)
- Generations may be defined by 100% replacement or by partial (overlapping x%) replacement.
- For policy, GA designers should also keep 1 or more best “champions” each generation, without changing them. This is so you never lose the best solution found so far.

GeoGraph Data Summary

		Nodes	Links	Air Travel Behaviour	Land Travel Behaviour
US	47 Cities	Yes (1)	Yes (3)	Yes (5)	Limited Data, Needs Special Processing
	250 Cities	Yes (1)	Yes (3)	Yes (5)	Limited Data, Needs Special Processing
World	250 Cities	Yes (2)	Yes (4)	Limited Data, Needs Special Processing	No Data
	500 Cities	Yes (2)	Yes (4)	Limited Data, Needs Special Processing	No Data
	1000 Cities	Yes (2)	Yes (4)	Limited Data, Needs Special Processing	No Data

1: US Census PHC-T-29, 2000 Data
http://www.census.gov/population/www/estimates/metroarea.html
2: World Gazetteer,
http://www.world-gazetteer.com/wg.php?x=1129315561&men=stdl&lng=en&gln=xx&dat=32&srt=npan&col=aohdq
3: BTS T100, 2003 Data (Q1-Q3) gathered by RTI; other periods available directly from BTS
https://www.epimodels.org/midas/metadata.do?method=view&referenceId=FINAL%20T-100%20Domestic%20Segment%2050%20Cities,
http://www.transtats.bts.gov/tables.asp?db_id=110&DB_Name=
4: OAG World Survey, Nov 2000 Data, gathered by RTI,
https://www.epimodels.org/midas/metadata.do?method=view&referenceId=OAG%20Flight%20Schedule%20Data%202000%20to%202001
5: BTS DB1B, 2004 Data,
http://www.transtats.bts.gov/TableInfo.asp?Table_ID=289&DB_Short_Name=Origin%20and%20Destination%20Survey&Info_Only=0\