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Introduction to Agent-based Modeling and Simulation

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The "Name Game"

- ABMS is known by many names:
  - ABM: "Agent-based modeling" or "anti-ballistic missile?"
  - ABS: "Agent-based simulation" or "anti-lock brakes?"
  - IBM: "Individual-based modeling" or "International Business Machines Corporation?"
- ABM, ABS, and IBM are all widely-used acronyms, but "ABMS" will be used throughout this discussion
- ABMS is not the same as "mobile agents"

The Need for Agent-based Modeling

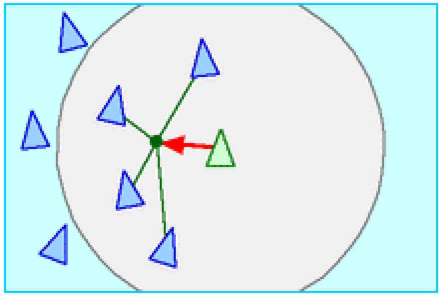
We live in an increasingly complex world.

- **Systems More Complex**
  - Systems that need to be analyzed are becoming more complex
  - Decentralization of Decision-Making: “Deregulated” electric power industry
  - Systems Approaching Design Limits: Transportation networks
  - Increasing Physical and Economic Interdependencies: infrastructures (electricity, natural gas, telecommunications)
- **New Tools, Toolkits, Modeling Approaches**
  - Some systems have always been complex, but tools did not exist to analyze them
  - Economic markets and the diversity among economic agents
  - Social systems, social networks
- **Data**
  - Data now organized into databases at finer levels of granularity (micro-data) – can now support micro-simulations
- **Computational Power**
  - Computational power advancing – can now support micro-simulations

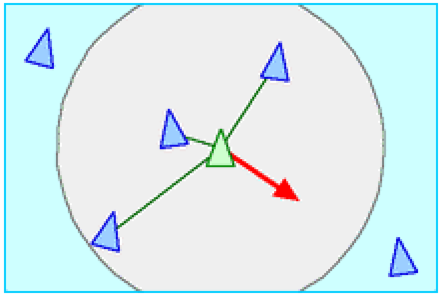
Agent-based Simulation Is a New Field Grounded in the Biological, Social, and Other Sciences

- What is an agent?
  - A discrete entity with its own goals and behaviors
  - Autonomous, with a capability to adapt and modify its behaviors
- Assumptions
  - Some key aspect of behaviors can be described.
  - Mechanisms by which agents interact can be described.
  - Complex social processes and a system can be built "from the bottom up."
- Examples
  - People, groups, organizations
  - Social insects, swarms
  - Robots, systems of collaborating robots
- Agents are diverse and heterogeneous

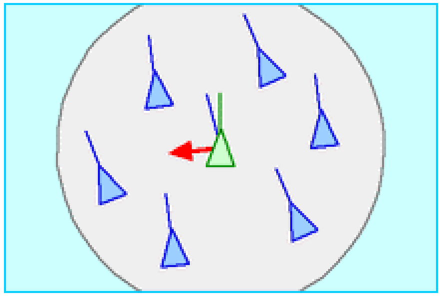
Example: Modeling Simple Schooling/Flocking Behavior with Agent Rules



Cohesion:
Steer to move toward the average position of local flockmates



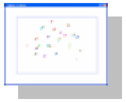
Separation:
Steer to avoid crowding local flockmates



Alignment:
Steer towards the average heading of local flockmates

Source: "Boids" by Craig Reynolds, http://www.red3d.com/cwr/boids/

Demonstration: Boids Model

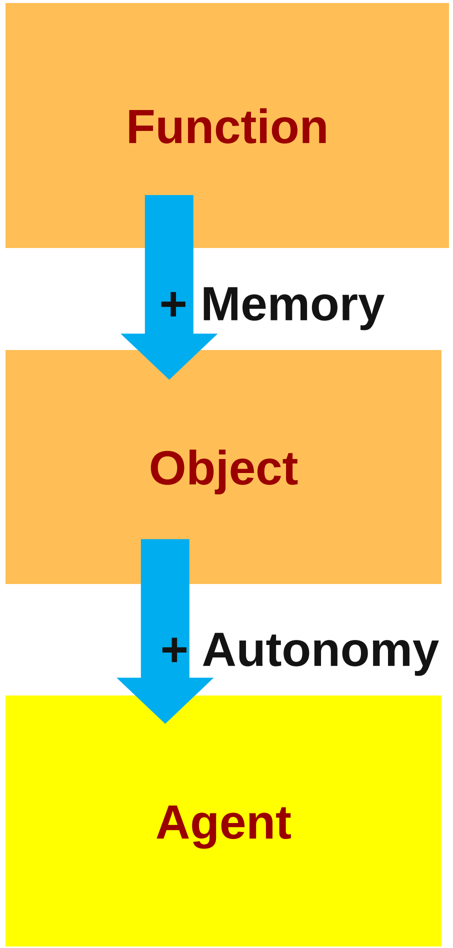


C:\Documents and Settings\macal\My Documents_myMathematica\(Model)\BoidsNeighborhoodAlgorithm-AnalyzeResults(09-14-06-1pm)

What Is An Agent? Agents Are Autonomous Decision-making Units with Diverse Characteristics (Heterogeneous)

- **Decision rules vary by agent**
  - Sophistication of rules
  - Cognitive “load”
  - Internal models of the external world
  - Memory employed
- **Agents vary by their attributes and available accumulated resources**
- **What is the effect of agent diversity on the system?**
  - Do certain types of agents dominate?
  - Does the system evolve toward a stable mix of agent types?

What Is an "Agent?"



Agent Simulation Is Based on "Local" Interaction Among Agents

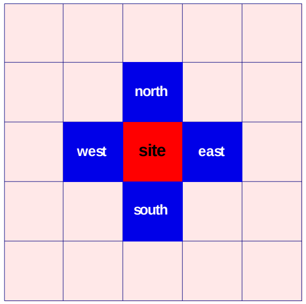
- No central authority or controller exists for:
  - How the system operates
  - How the system is modeled
  - How the system/model moves from state to state
- "Optimization" can be done for the system as a whole

Agent Interaction Topologies: Agents Have Neighborhoods

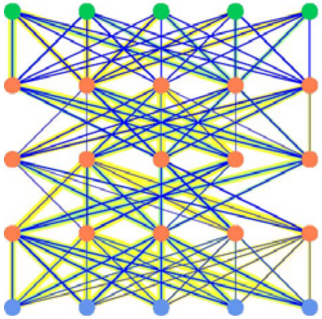
Various Topologies Connect Agents with Their Neighbors

- Agents can move in free (continuous) space
- Cellular automata have agents interacting in local "neighborhoods"
- Agents can be connected by networks of various types and be static or dynamic
- Agents can move over Geographical Information Systems (GIS) tilings
- Sometimes *spatial* interactions are not important ("Soup" Model)

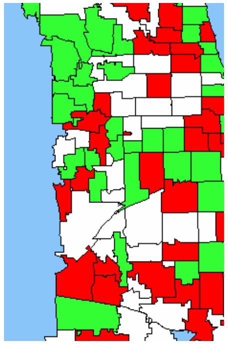
Euclidean Space: *2D, 3D*



Grid: *von Neumann neighborhood*



Network



GIS: Geographic Information System

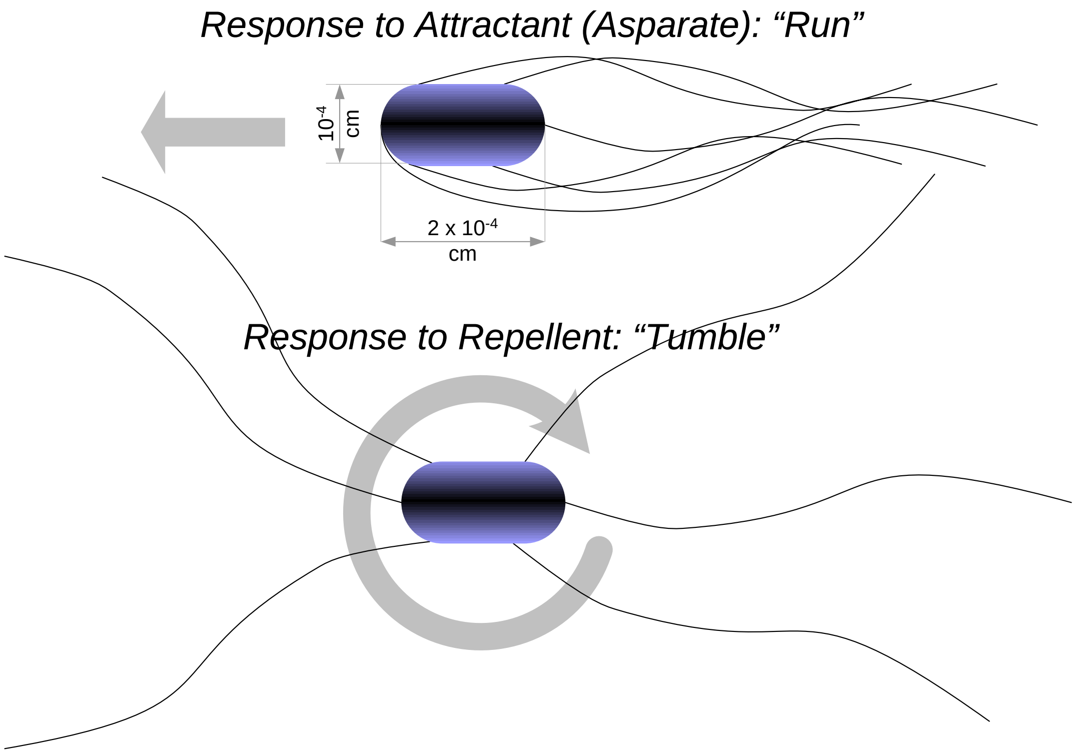
Application: Bacterial Chemotaxis

- **Motivation:** In recent years, single-cell biology has focused on the relationship between the stochastic nature of molecular interactions and variability of cellular behavior.
  - To describe this relationship, it is necessary to develop new computational approaches at the single-cell level.
- **Results:** We have developed *AgentCell*, a model using agent-based technology to study the relationship between stochastic intracellular processes and behavior of individual cells.
  - As a test-bed for our approach we use bacterial chemotaxis, one of the best characterized biological systems.
  - In this model, each bacterium is an agent equipped with its own chemotaxis network, motors and flagella.
  - Swimming cells are free to move in a 3D environment.

Application: Linking Chemical Reaction Networks to Behavior

Simulating bacterial chemotaxis allows us to understand the fundamental biochemical processes of all living things

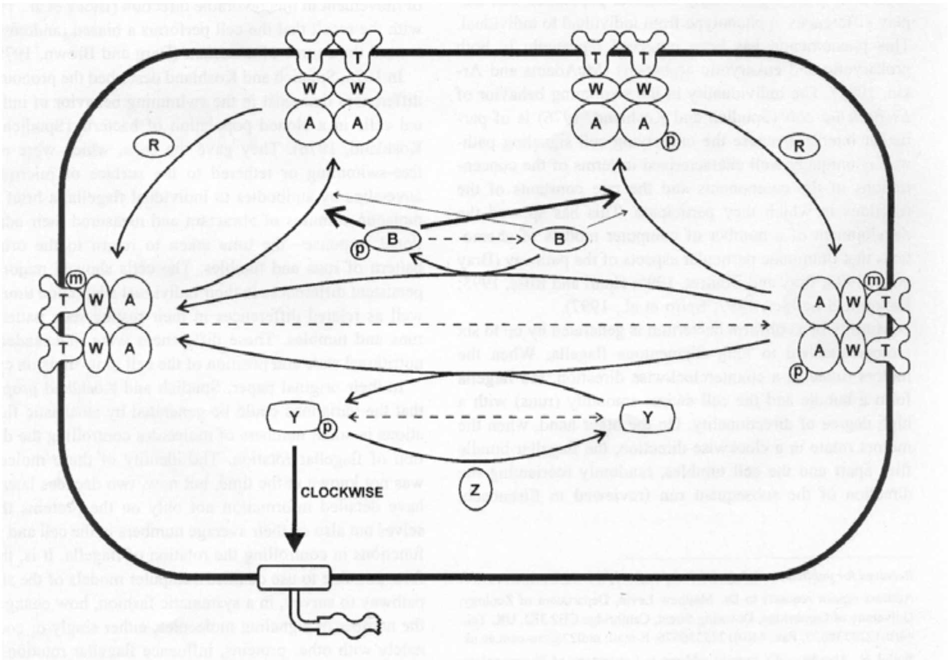
Motility of *Escherichia Coli*



Agent: Cell

- **Attributes:** Size
- **Rules of behavior:**
  - Natural motile behavior
  - Movement in response to stimuli
- **Memory: ???**
- **Sophistication:**
  - Interpret chemical signatures from other cells?
- **Resources: ???**

E.Coli *Signal Transduction Pathways*



- **Chemical pathway consists of transmembrane receptor proteins (e.g.,** Tar) **and products of four chemotaxis genes:** CheW, CheA, CheY, CheZ
- **Proteins convey information on binding of attractants or repellents at receptors to flagella motor, and modify the direction of its motor**
- **Receptors are bound in a complex to** CheA **via** CheW
- **Phosphoryl groups transferred from phosphorylated** CheA**,** CheAp**, to** CheY
- **Phosphorylated** CheY**,** CheYp**, diffuses to switch complex of the motor**

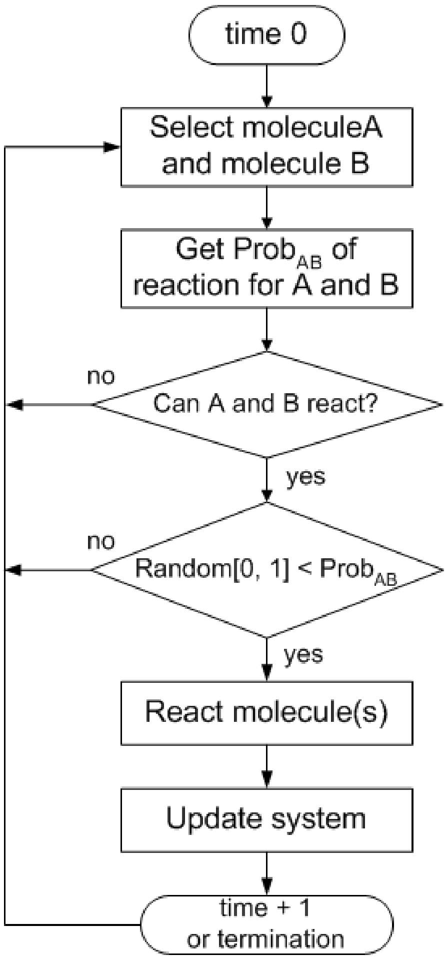
Ref: Levin, M., C. Mortin-Firth, W. Abouhamad, R. Bourrret, D. Bray, 1998, "Origins of individual swimming behavior in bacteria," *Biophysical Journal*, **74**: 175-181.

Modeling Problem #1: Signal Transduction
The Discrete Stochastic Simulation Approach

- Every molecule modeled individually
- Select molecules at random and determine whether reaction occurs
- Prob[A reacts with B]

$$= \frac{k_2 \times n\,(n + n_0) \times \Delta t}{2 \times N_A \times V}$$

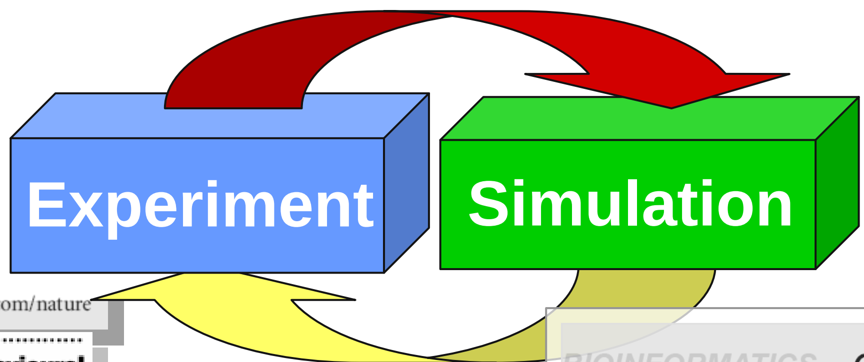
n = number of molecules in system
n_0 = number of pseudo-molecules in system
k_2 = molecular rate constant ($M^{-1}s^{-1}$)
Δt = time slice duration (s)
N_A = Avogadro constant
V = volume of system (l)

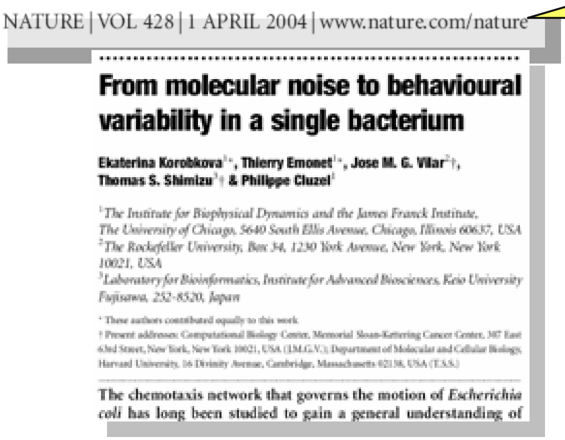


Ref: Firth, C., N. Le Novere, and T. Shimizu, 2002, "StochSim, the STOCHastic SIMulator".

Agent-based Simulation Relates Characteristics of the Observed Behavior with Network Architecture

- First build an agent-based network that can reproduce some of the key properties of the chemotaxis network
- Validate model by comparing results of numerical simulations with lab data
- Use the flexibility of agent-based modeling to study the modular structure of the chemotaxis network and of signal transduction networks in general





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From molecular noise to behavioural variability in a single bacterium

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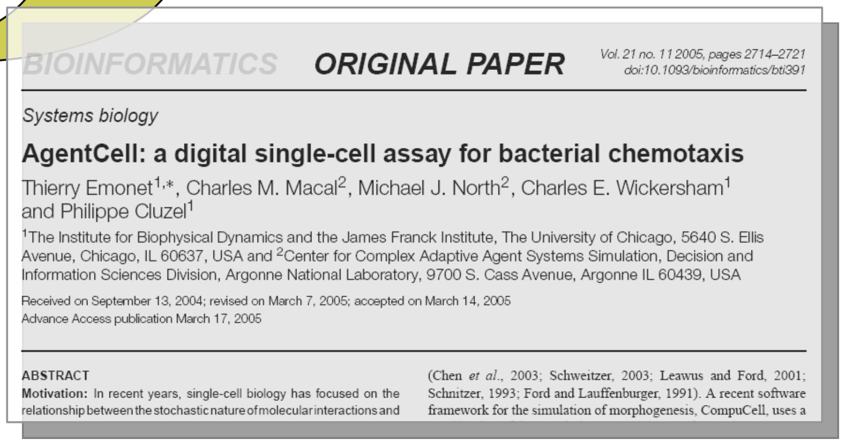
The chemotaxis network that governs the motion of *Escherichia coli* has long been studied to gain a general understanding of



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Systems biology

AgentCell: a digital single-cell assay for bacterial chemotaxis

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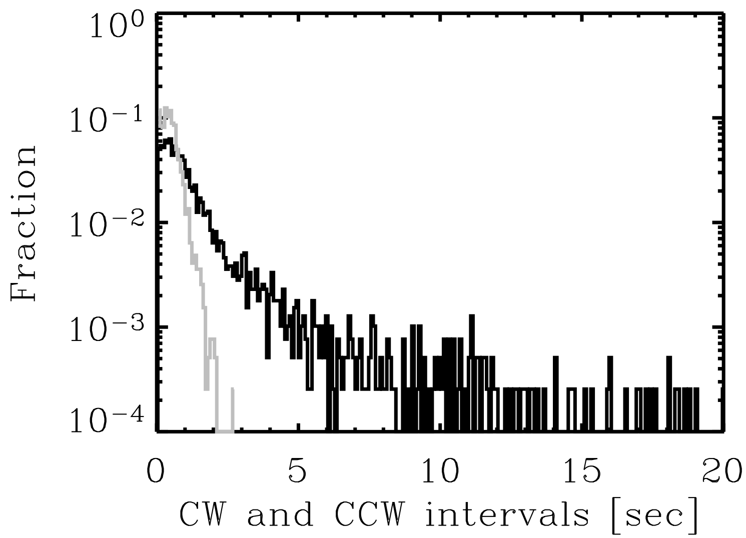
ABSTRACT
Motivation: In recent years, single-cell biology has focused on the relationship between the stochastic nature of molecular interactions and

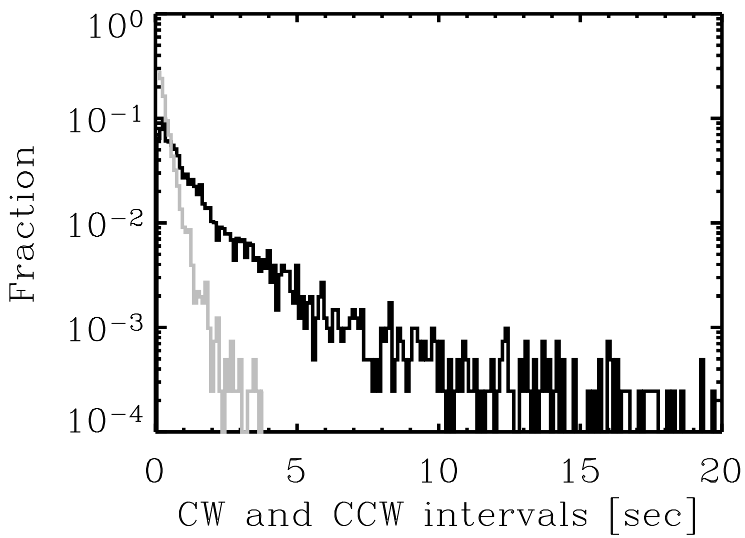
(Chen *et al.*, 2003; Schweitzer, 2003; Leawus and Ford, 2001; Schnitzer, 1993; Ford and Lauffenburger, 1991). A recent software framework for the simulation of morphogenesis, CompuCell, uses a

Using AgentCell digital chemotaxis assays reproduce experimental data obtained from both single cells and bacterial populations.

(a) ***experimental laboratory data*** on the distribution of CW (cell spins in place) and CCW (cell runs in a direction) intervals obtained by monitoring the switching events of individual cell flagella motors.



(b) ***simulated cell data*** on distribution of CW and CCW intervals resulting from the states of the motor in one of the cells in our digital population.



Architecture of AgentCell

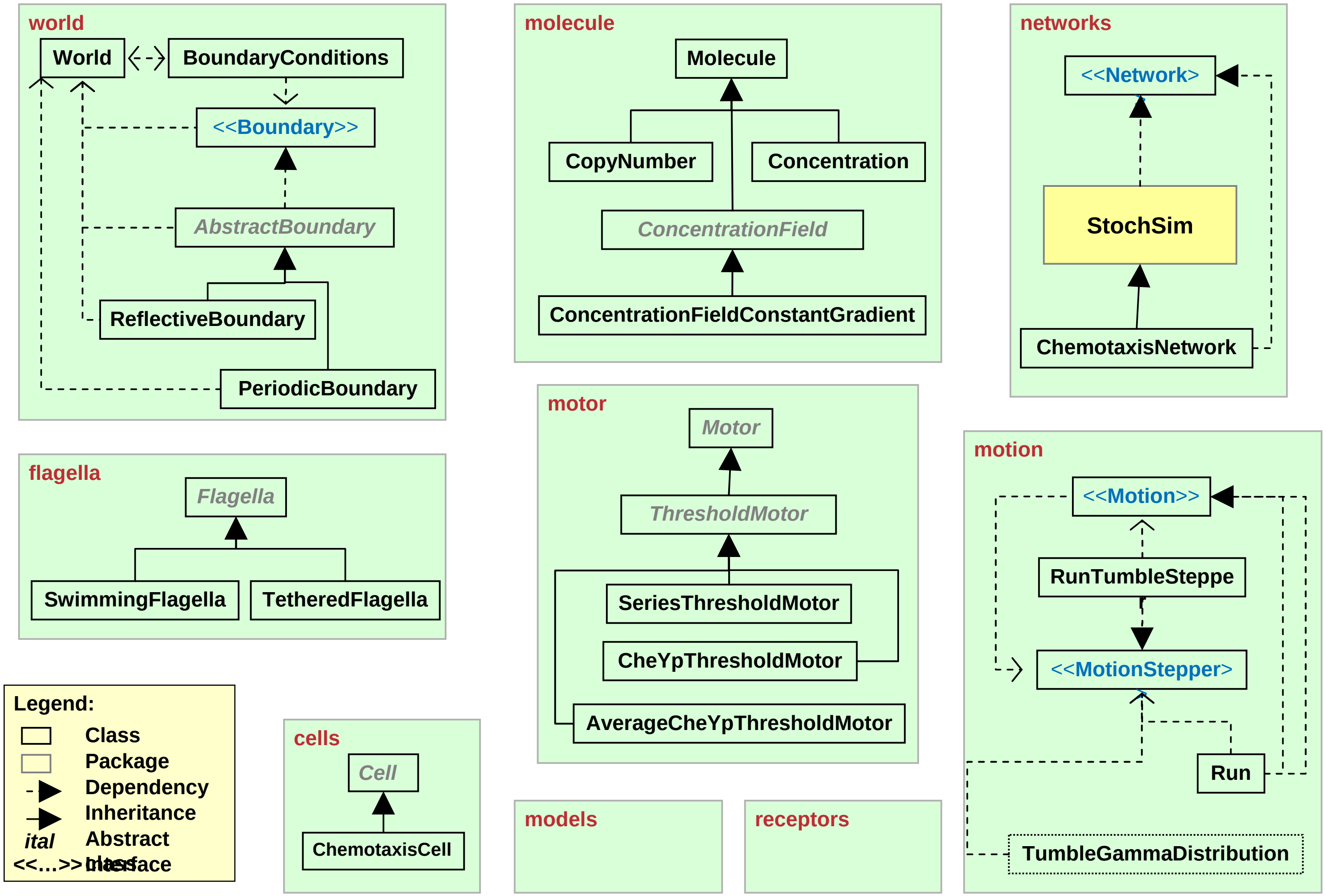
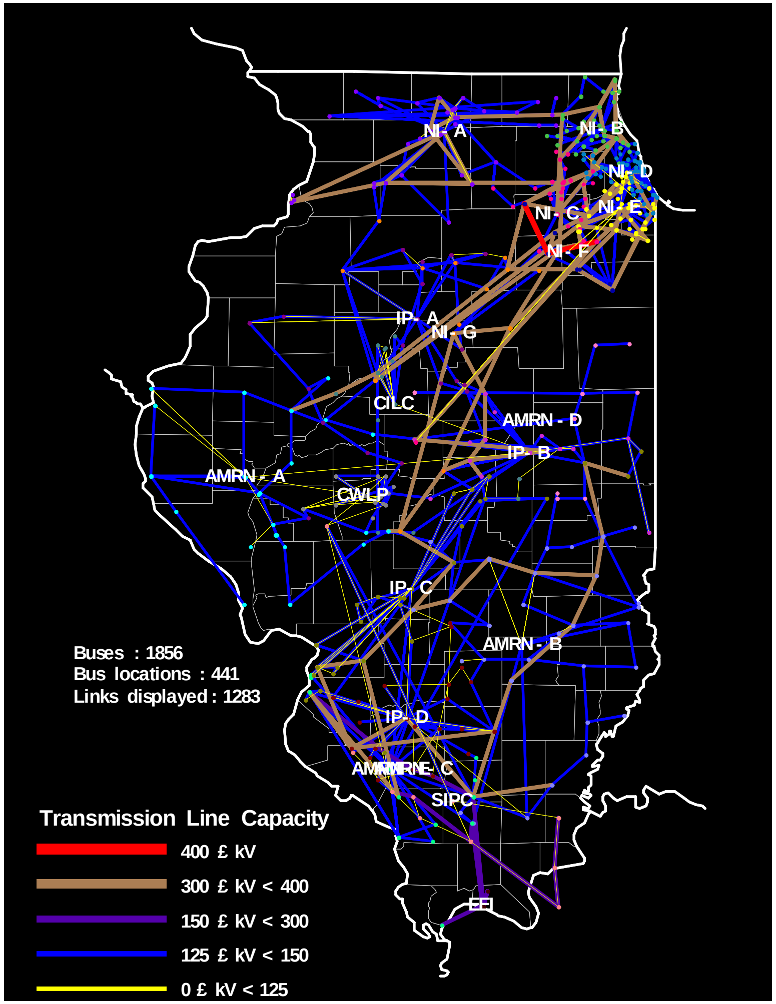
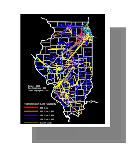


Fig. 1 Architecture of *AgentCell*: Class diagram showing the inheritances and dependencies between the main classes. Packages group together closely related classes.

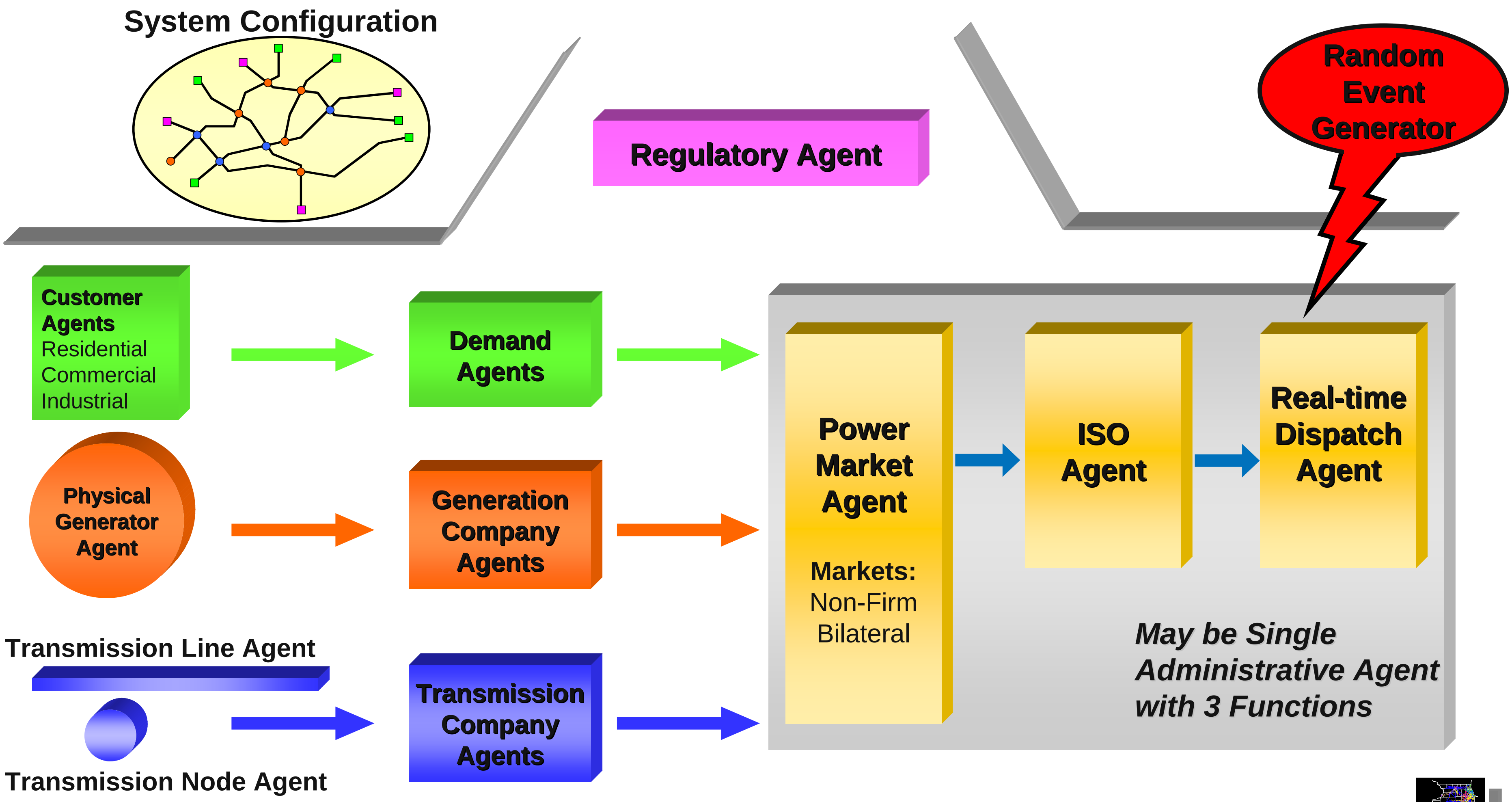
Large-Scale ABMS:
Application: Electric Power Markets
How will Illinois fare under electricity deregulation: Jan. 1, 2007?

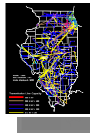


- Will power transmission capacity be adequate, or is congestion likely? Under what conditions?
- Will transmissions constraints on the power grid create regional imbalances in supply and demand?
- Will imbalances create pockets of market power and potentially drive up locational electricity prices?

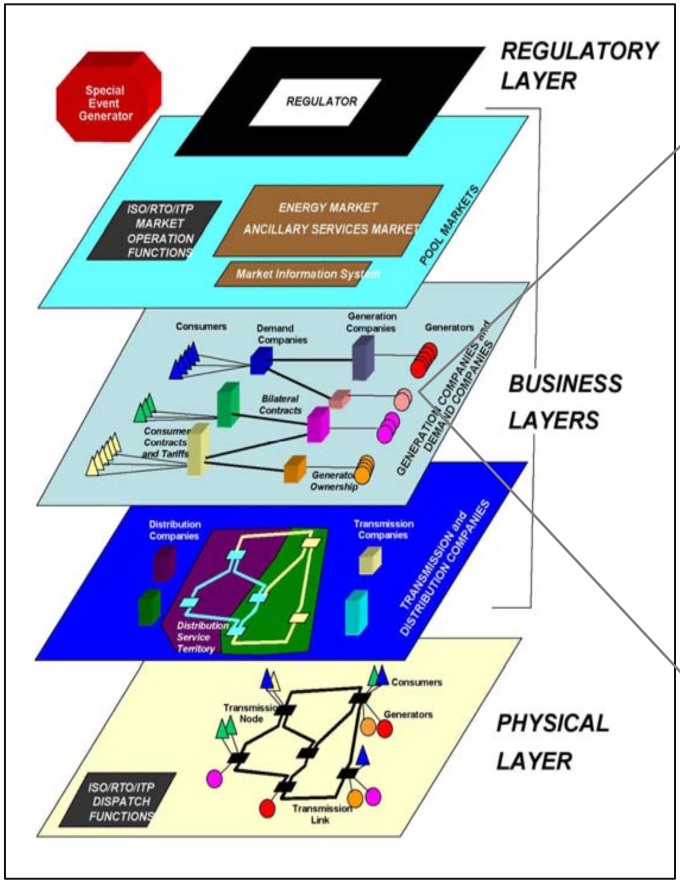


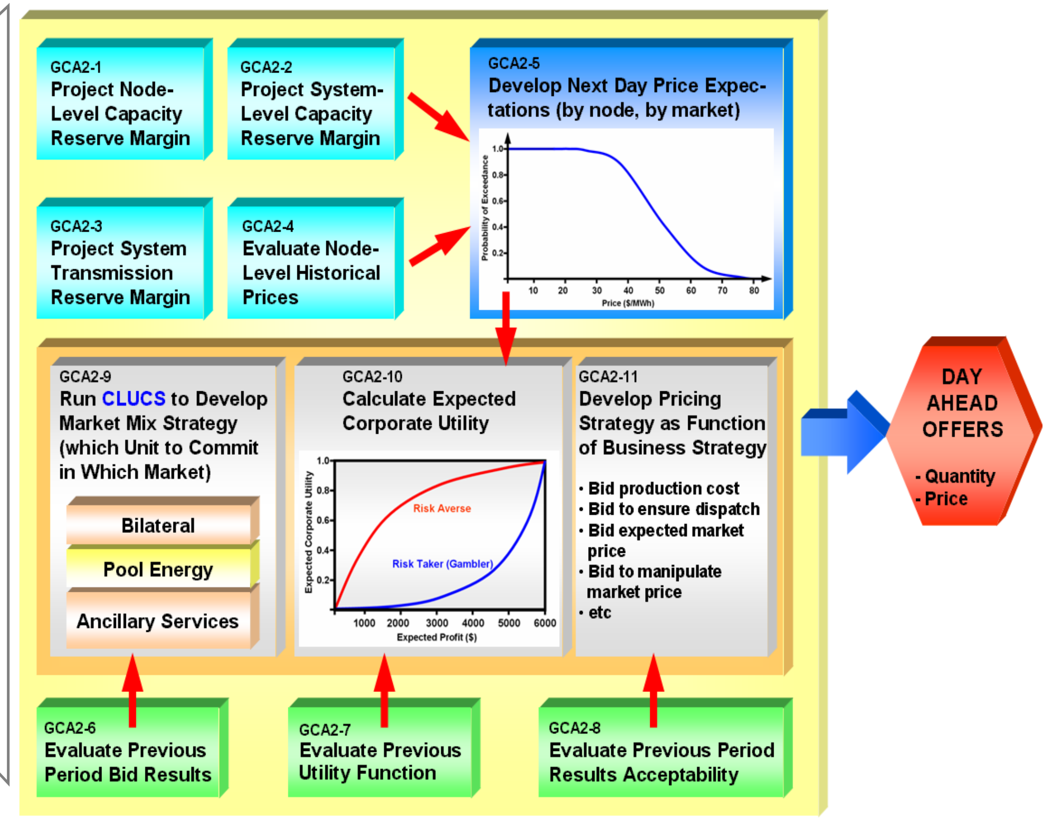
EMCAS Uses an Agent-Based Architecture to Represent the New Marketplace





Generation Company Agents Consider Many Factors in Proposing Bids for the Day-Ahead Market





Cases Were Constructed as "Electronic Experiments" to Study Market Behavior

Production Cost	**•Generation companies bid production cost** **•Gives the lowest system cost**
Physical Withholding	**•Intentionally take generators out of service** **•Prices rise**
Economic Withholding	**•Generation companies bid above production cost** **•Prices rise**

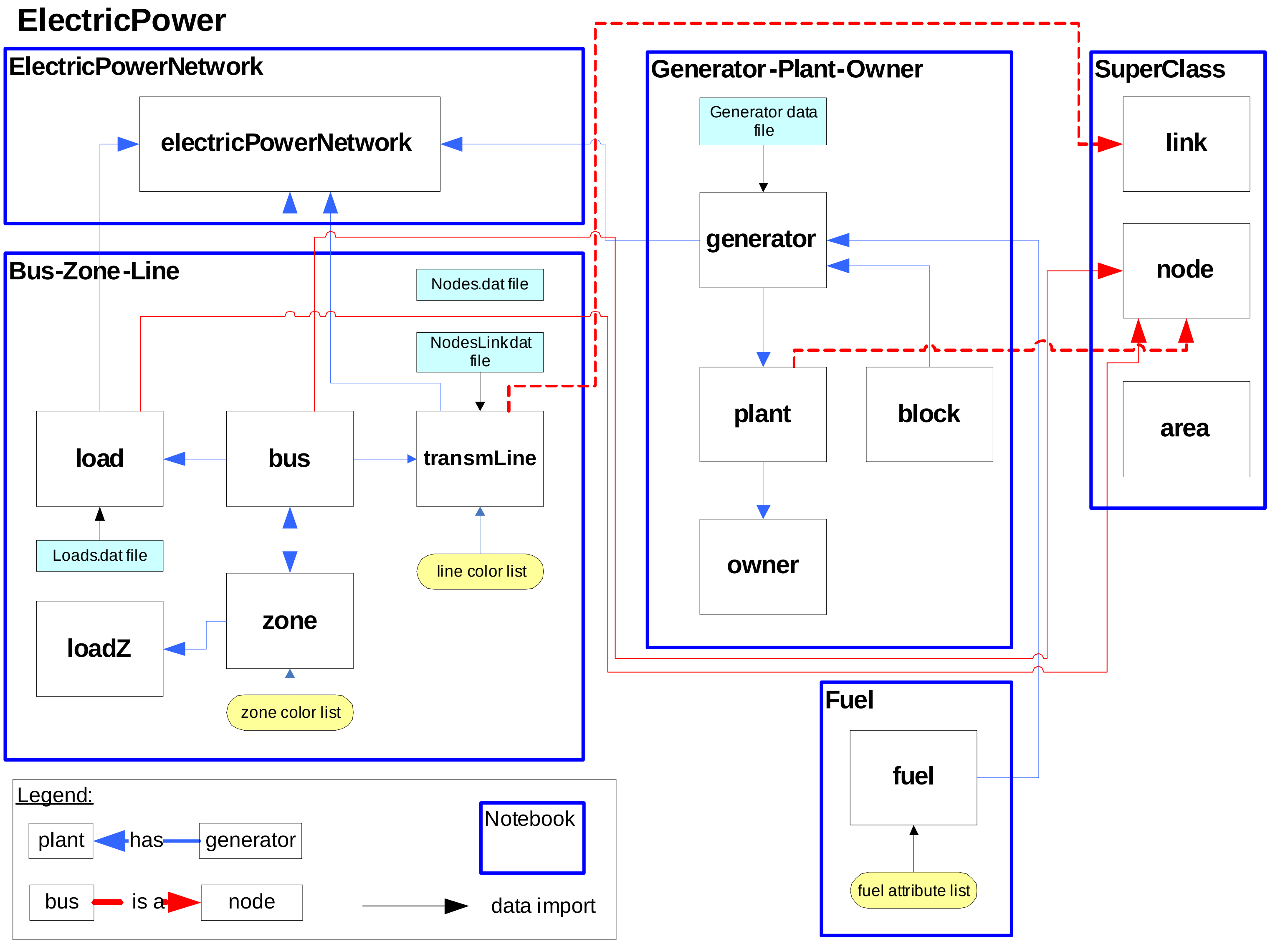
•Experiments moved from very simple to more complex strategies

•Production Cost Case used as a benchmark

•Not intended to imply that any company would attempt to exercise market power

•Only an initial mapping of possible market bidding

Architecture of EMCAS



EMCAS Impact

- The findings: *There is the potential for some companies to exercise market power (i.e., raise prices and increase profitability by unilateral action) and raise consumer costs under selected conditions, particularly when there is transmission congestion.*
- EMCAS results* have been entered into the public record of the Illinois Commerce Commission (ICC), 6 June 2006.
- Report available from the ICC web site http://www.icc.illinois.gov/
- EMCAS is an example of an agent-based model that has been successfully applied to a real-world policy issue and provided information that would otherwise have not been available using any other modeling approach.

*Cirillo, R., P. Thimmapuram, T. Veselka, V. Koritarov, G. Conzelmann, C. Macal, G. Boyd, M. North, T. Overbye and X. Cheng. 2006. *Evaluating the Potential Impact of Transmission Constraints on the Operation of a Competitive Electricity Market in Illinois*, Argonne National Laboratory, Argonne, IL, ANL-06/16 (report prepared for the Illinois Commerce Commission), April.

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What Is Agent-Based Modeling & Simulation?

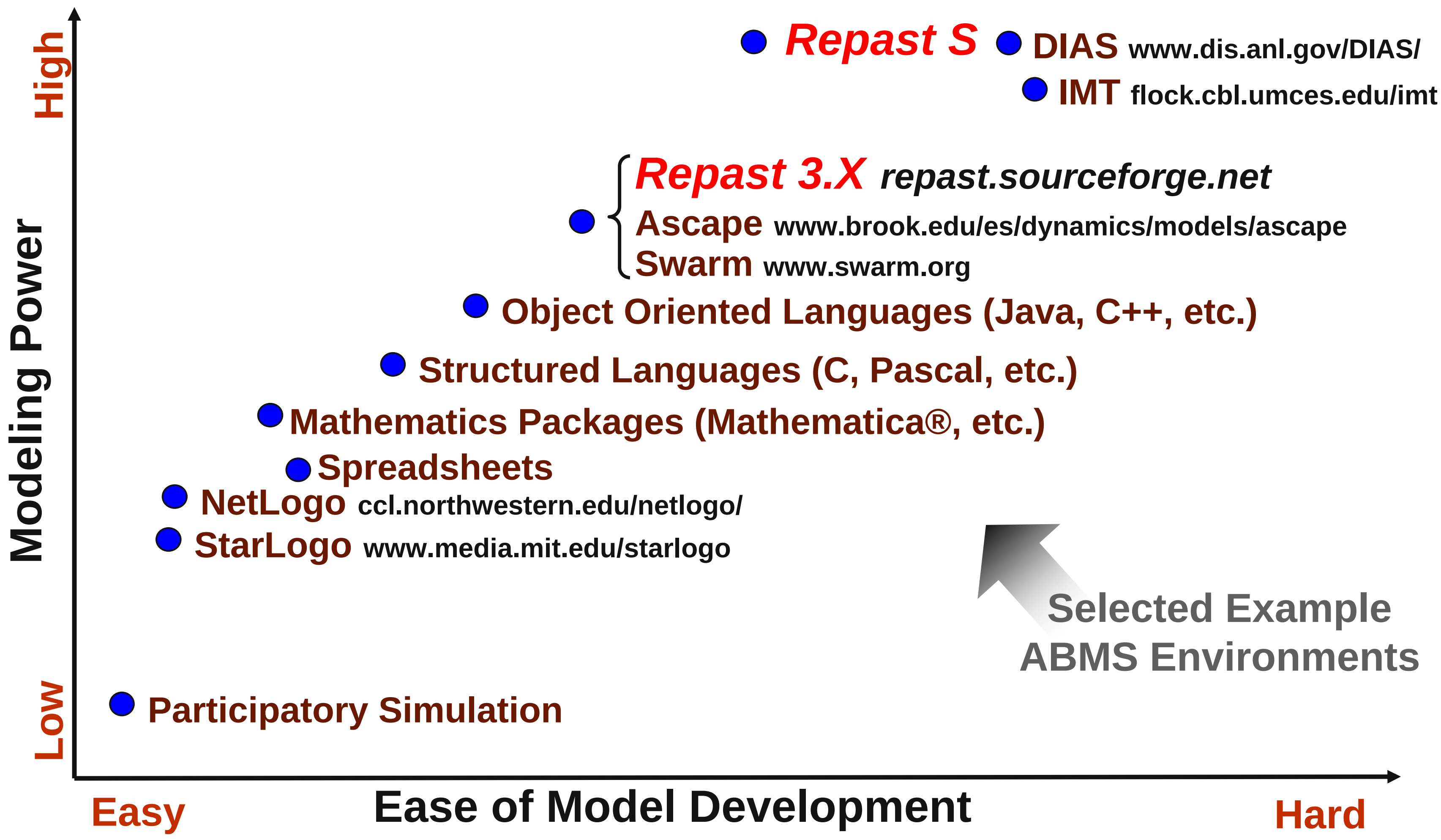
- An agent-based model consists of:
  - A set of agents (part of the user-defined model)
  - A set of agent relationships (part of the user-defined model)
  - A framework for simulating agent behaviors and interactions (provided by an ABMS toolkit or other implementation)
- Unlike other modeling approaches, agent-based modeling begins and ends with the agent's perspective

ABMS Platforms

- Agent-based Modeling and Simulation Toolkits
  - Repast (Java) – similar to Swarm (Objective C, Java)
  - NetLogo, StarLogo
  - MASON
  - AnyLogic (commercial)
- General Tools
  - Spreadsheets, with macro programming
  - Computational Mathematics Systems
    - MATLAB
    - *Mathematica*
  - General Programming Languages (Object-oriented)
    - *Java*
    - *C++*

The agent-based model development process often makes use of several tools.

ABMS Uses Specific Tools



EMCAS and AgentCell Are Based on Repast

- *Repast* (Recursive Porous Agent Simulation Toolkit) is a free and open source agent modeling toolkit under continual development by Argonne (Repast was originally developed at the U of Chicago)
- Can be thought of as a specification for agent-based modeling services or functions
- Seeks to support the development of extremely flexible models of living social agents
- Provides an integrated set of libraries for neural networks, genetic algorithms, social network modeling, and other topics
- Available in pure Java and pure Microsoft.Net forms:

  http://repast.sourceforge.net/

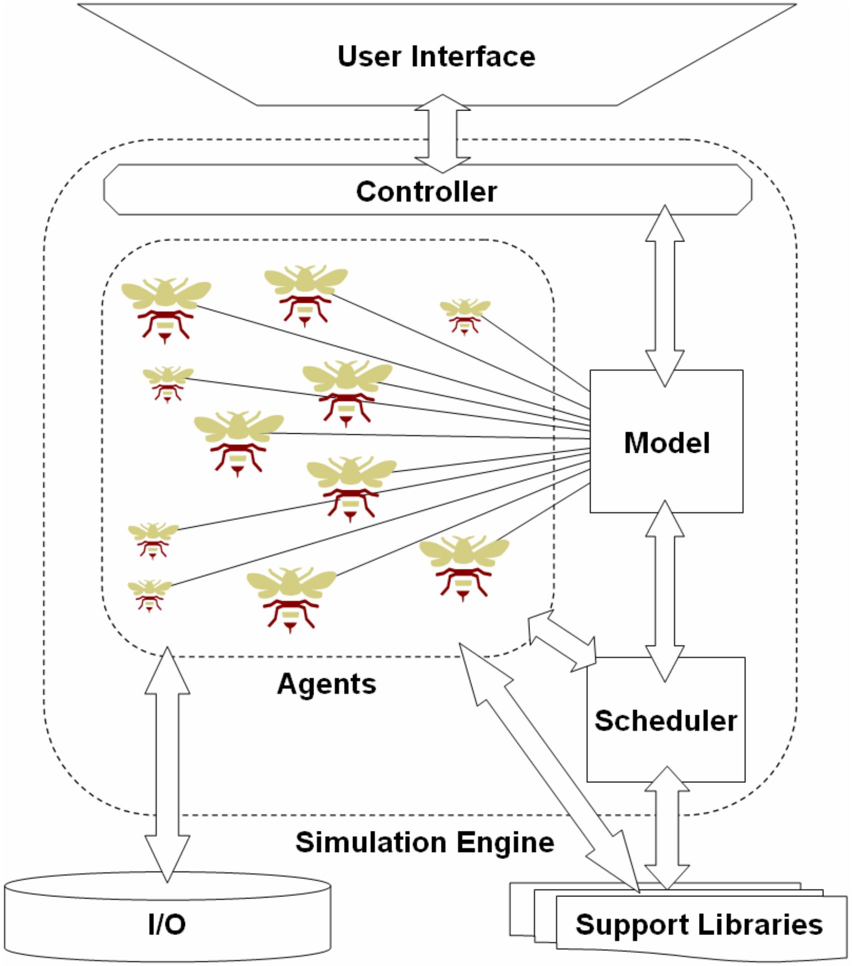
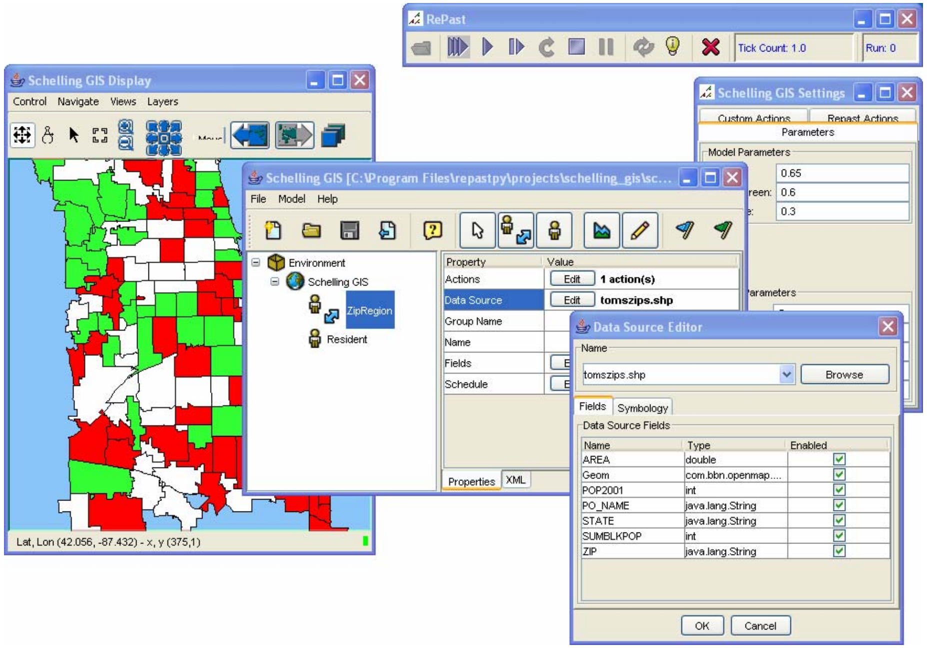


Fig. 7. Repast Overview Diagram

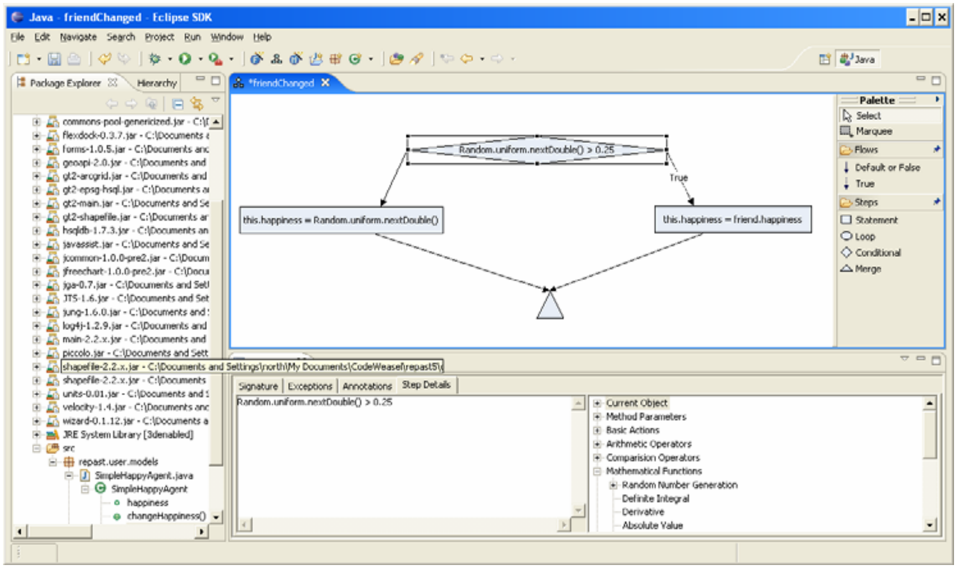
The REcursive Porous Agent Simulation Toolkit (Repast): A free, open source ABMS toolkit

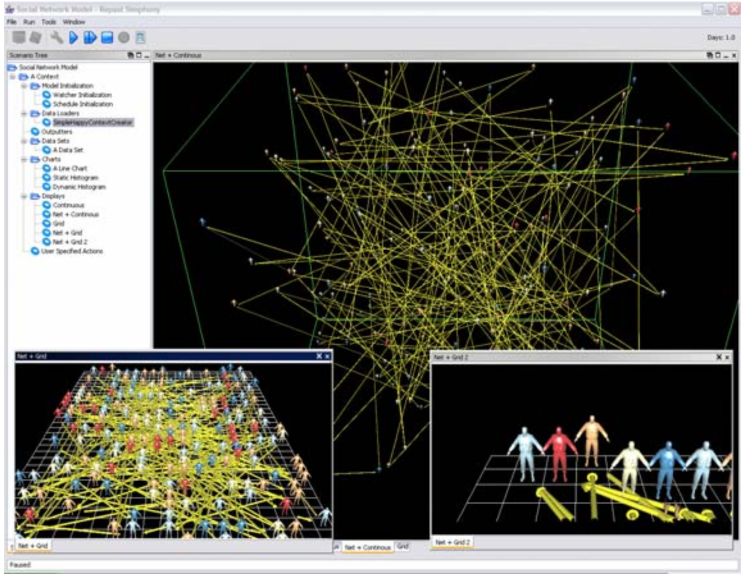
- Repast is available in pure Java and pure Microsoft.NET C# framework forms:
  - Repast Simphony (Repast S)
  - Repast for Java (Repast J)
  - Repast for Microsoft .NET framework (Repast .NET)
  - Repast for Python Scripting (Repast Py)
  - Repast Agent Analyst for ESRI ArcGIS
- Repast focuses on social simulation, but can be used for any domain



This is Repast Simphony (Repast S)

- Repast S is useful for both beginning and experienced modelers
- Repast S includes many features:
  - Visual model development
  - Point-and-click model configuration and operation
  - Integrated 2D, 3D, GIS, and narrative model views
  - Automated connections to enterprise data sources such as relational databases and GIS
  - Automated connections to powerful external programs for statistical analysis and visualization of model results



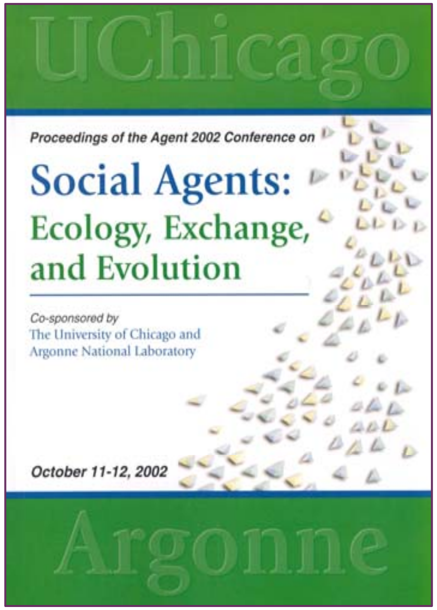


When agent modeling?

- When there is a natural representation as agents
  - When there are decision and behaviors that can be defined discretely (with boundaries)
  - When it is important that agents adapt and change their behavior
  - When it is important that agents learn and engage in dynamic strategic behavior
  - When it is important that agents have a dynamic relationships with other agents, and agent relationships form and dissolve
  - When it is important that agents form organizations and adaptation and learning are important at the organization level
  - When it is important that agents have a spatial component to their behaviors and interactions
- When the past is no predictor of the future
- When scale-up to arbitrary levels is important
- When process structural change needs to be a result of the model, rather than an input to the model

As a Note, Argonne Sponsors a Conference and a Training Course to Promote CAS Development and Applications

ABMS 2007: 5-day Course on Agent-Based Modeling & Simulation, with *Santa Fe Institute,* April 2007, Argonne National Lab IL



Agent 2007: Challenges in Social Agent Simulation, with *University of Chicago,* August 16 - 18, 2006, Chicago

Questions?

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The End

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