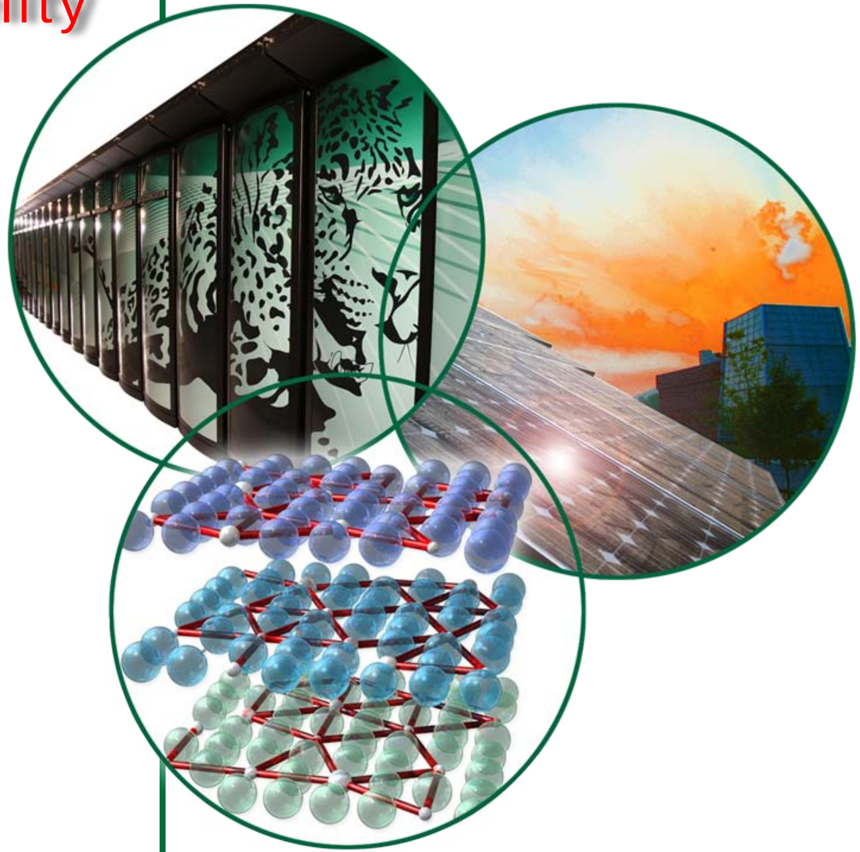
High-Performance Simulations of Complex Networked Systems
for Capturing Feedback and Fidelity

SIAM PP Conference, Seattle

Feb 26, 2010



Kalyan S. Perumalla, Ph.D.

Senior Research Staff Member
Oak Ridge National Laboratory

Adjunct Professor
Georgia Institute of Technology

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Main Thesis

Model Feedback and Fidelity

- Feedback is appearing as essential in recent models
  - Across a range of domains and applications
- Feedback seems to necessitate higher fidelity
  - To integrate phenomena with network dynamics

Implications to Computation

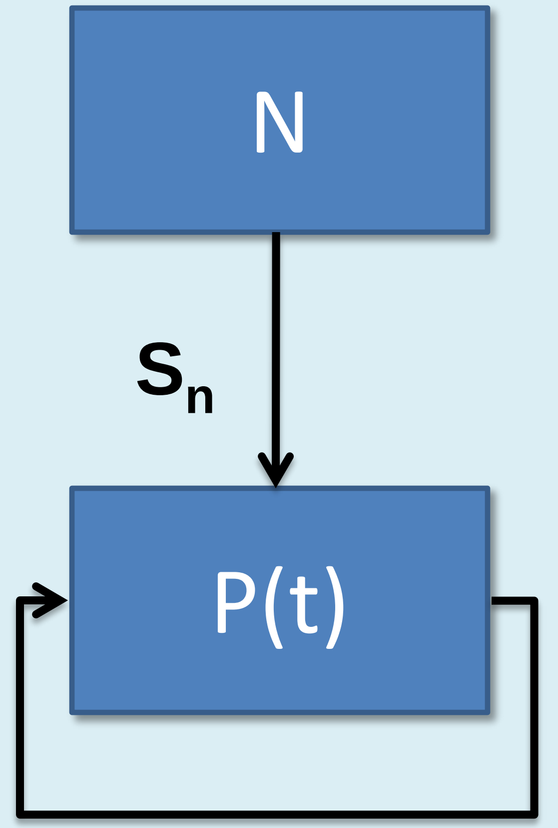
- Computation needs overall are dramatically increased
  - To simulate new models
  - E.g., $O(N)$ to $O(N^2)$, $O(N^2)$ to $O(N^3)$
- High performance computing seems necessary
  - For fast simulation of feedback-heavy, high-fidelity models

Static Networks

Abstraction of Elements

- N : Network properties
  - Connectivity structure
  - E.g., Internet, roads, contacts
- P(t) : Phenomena of focus
  - E.g., entity movement, device state, cognitive attributes

Static Network Relation

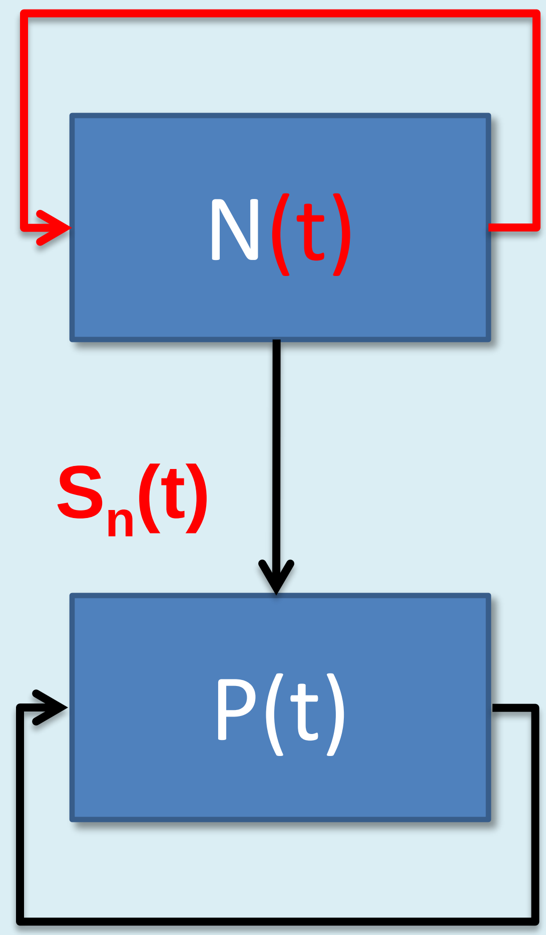


Dynamic Network without Feedback

Abstraction of Elements

- N(t) : Network properties
  - Structure, behavior
  - E.g., Traffic signals, packet store-forward, electric frequency
- P(t) : Phenomena of focus
  - Similar to previous (static)
  - Or slightly more refined/complex
- $S_n(t)$: State of network
  - Needed for P(t) dynamics
  - E.g.,

Dynamic-Network Relation

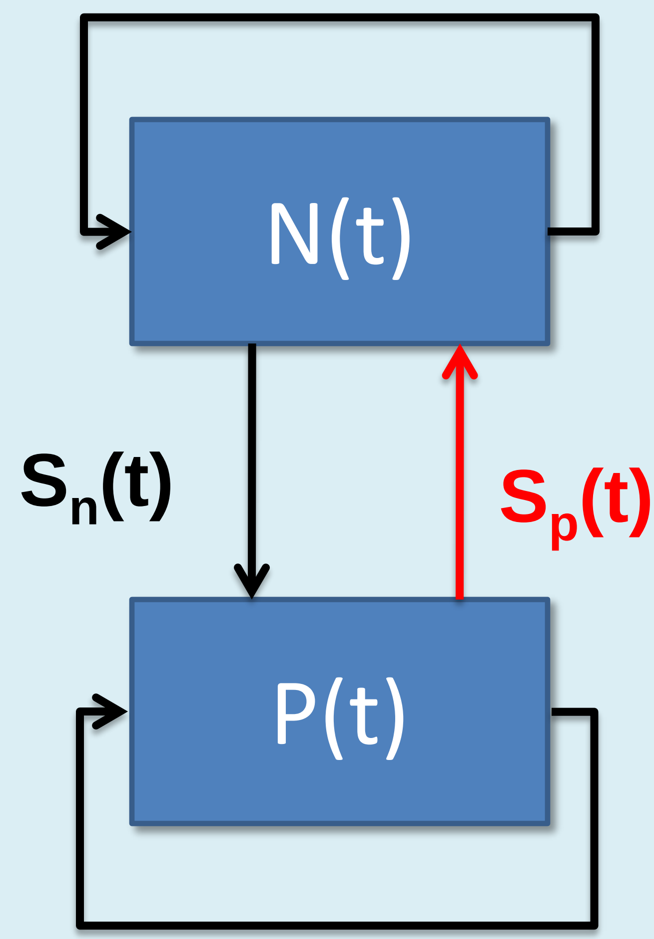


Feedback in Networked Systems

Abstraction of Elements

- N(t) : Network dynamics
  - Structure, behavior, reactions, coupling
- P(t) : Phenomena of focus
  - More tightly integrated operation
  - E.g.,
- $S_n(t)$: State of network
  - Needed for P(t) dynamics
- $S_p(t)$: State of phenomenon
  - "Feedback" of P(t) into N(t)

Nature of Feedback



Feedback-Heavy Networks: Illustrations

Simulation Domains	Feedback examples
• Cyber security Simulations	• E.g., bandwidth-limited worms
• Transportation Simulations	• E.g., dynamic re-routing
• Epidemiological Simulations	• E.g., quarantines and curfews
• Electric Grid Simulations	• E.g., smart grid devices
• *Several other, emerging domains*	• E.g., online-pricing, peer-to-peer networks

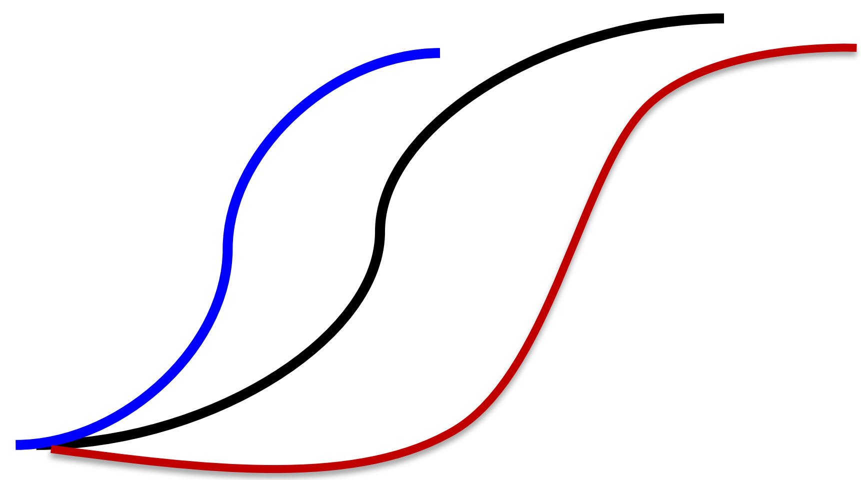
Example: Disease or Worm Propagation

SI Model

- Typical dynamics model
  - Multiple variants exist (e.g., SIR)
- Excellent fit
  - But *post-facto* (!)
  - Plot collected data
- Difficult as predictive model
  - Great amount of detail buried in α
- Feedback for accuracy
  - Interaction topology
  - Resource limitations
  - E.g., bandwidth-limited worm

P(t)

$$\frac{dI}{dt} = \alpha I(S - I)$$

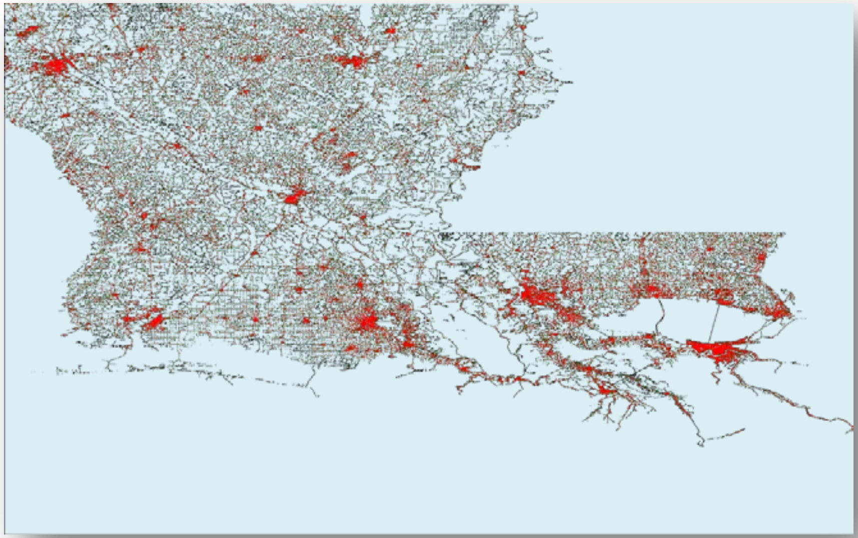


Transportation - Example

Dynamic, semi-automated rerouting

- Dynamic decisions
  - Individual-level
  - Semi-automated
  - Fairly tight feedback
- Vastly higher computational load
  - Shortest path per individual
  - Hard to aggregate
  - Poorly understood (analytically)
- Fundamental in nature
  - Needs duplication of M real computing units on fewer simulation computer's units

Evacuation time estimation or Emission control analysis



Transportation – Our Approach

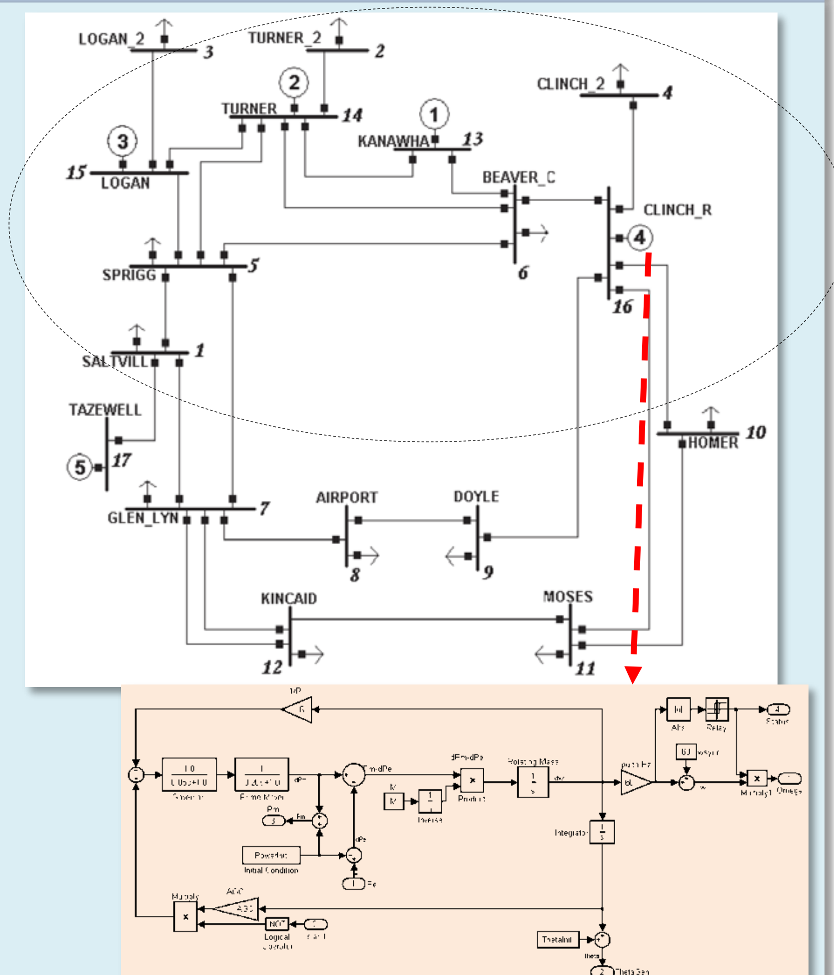
- SCATTER
  - “A Systems Approach to Scalable Vehicular Mobility Models,” Winter Simulation Conference ’06
  - “Kinetic and Non-Kinetic Aspects…,” Europen Modeling and Simulation Symposium ‘06
- Large-scale parallel discrete event simulation
- Efficient, cache-based on-demand shortest path computations

Electric Grid

Smart Grid

- Simulation-based analysis indispensible
- Feedback absolutely essential
- Fidelity of grid model must be elevated
- Computational load is dramatically increased

Smart Devices and Appliances



Electric "Smart" Grid – Our Approach

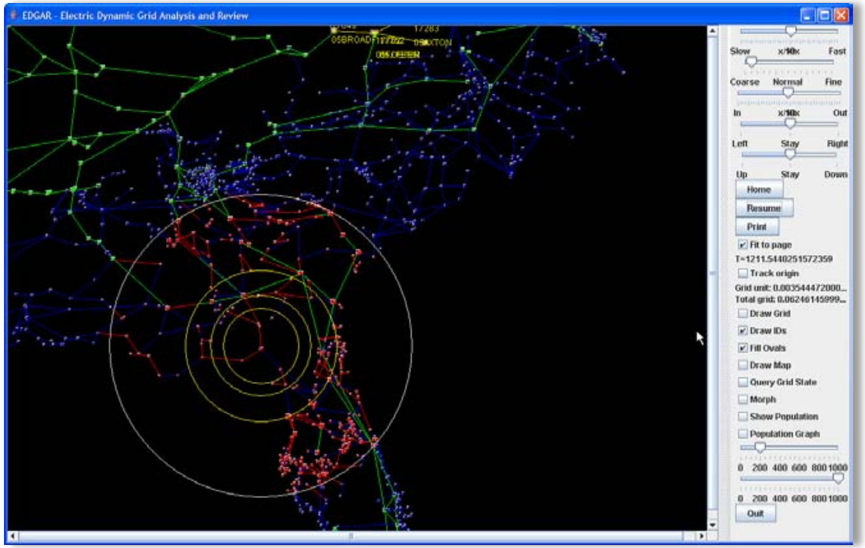
Discrete Event Formulation

- Detect threshold crossings at devices
- Evolve state of phenomenon P (electric)
  - Conventional equations
  - Coupled differential equations
- Incorporate network changes at threshold crossings
- Very heavy computation
  - Detection of crossings
  - Revision of network

Conventional (static): $O(n^2)$

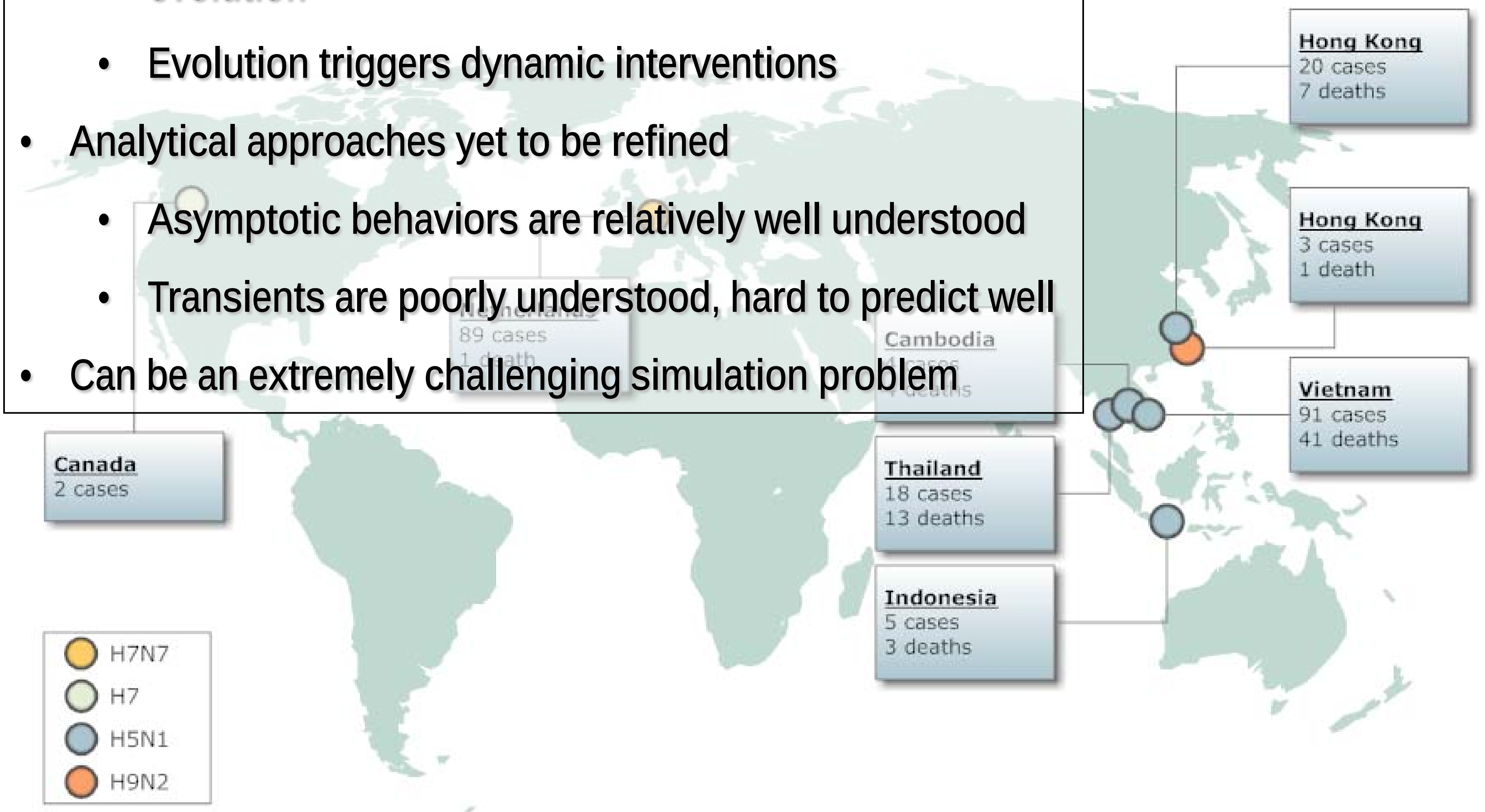
New (dynamic): O(n3)

n is large ~ 10^4 buses



Epidemiology – Feedback Example

- Network structure dictates *and is defined by* evolution
  - Interventions change network structure, in turn evolution
  - Evolution triggers dynamic interventions
- Analytical approaches yet to be refined
  - Asymptotic behaviors are relatively well understood
  - Transients are poorly understood, hard to predict well
- Can be an extremely challenging simulation problem



Epidemiology – Our Approach

- Optimistic parallel simulation
  - Cray XT5, Blue Gene P
- Reverse computation for efficient simulation
  - New discrete event formulation
  - Support dynamic decisions
  - Quarantines, curfews, closures, vaccinations
- "Switching to High Gear…"
  - Distributed Simulations and Real-time Applications '09
- Additional recent work to appear soon

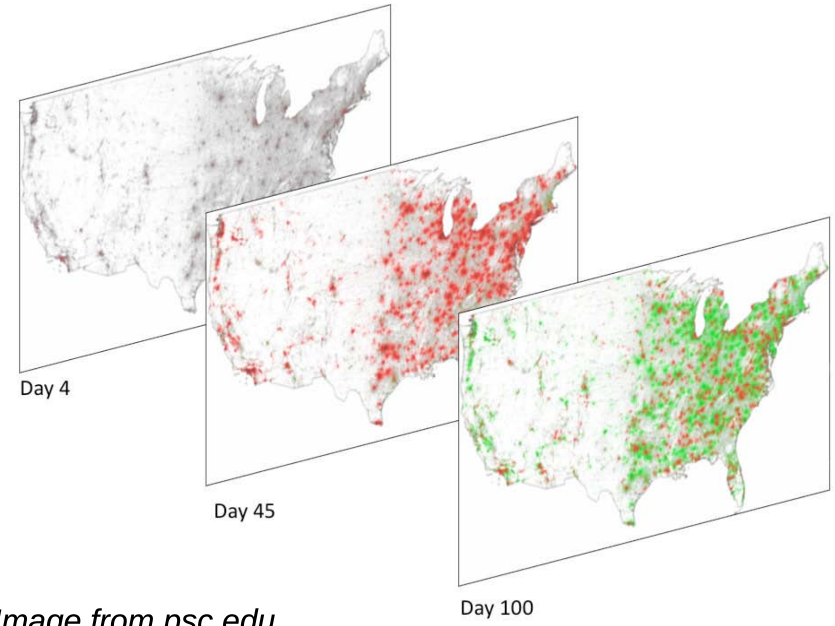
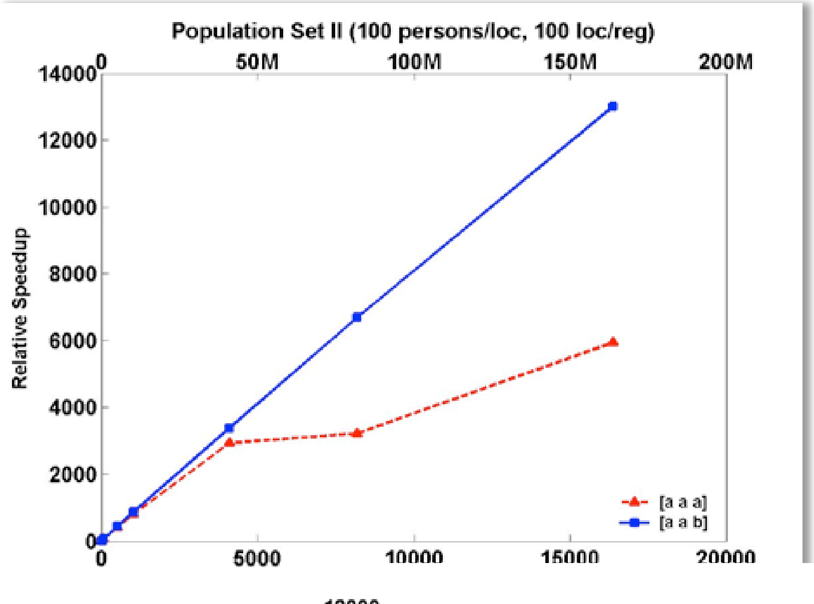
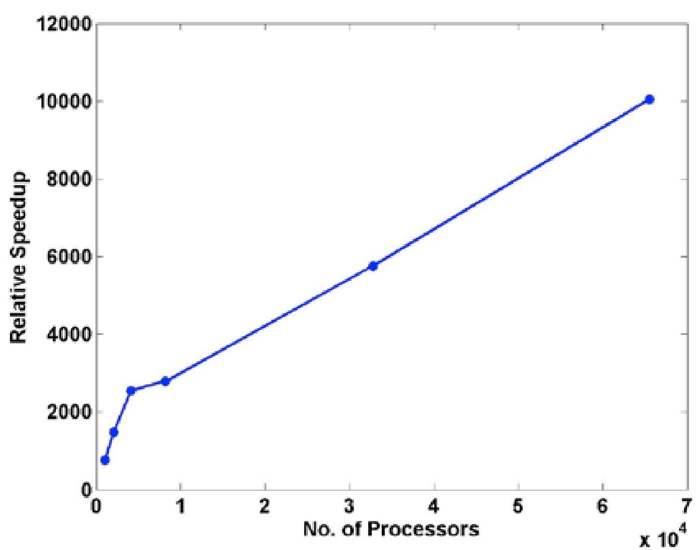
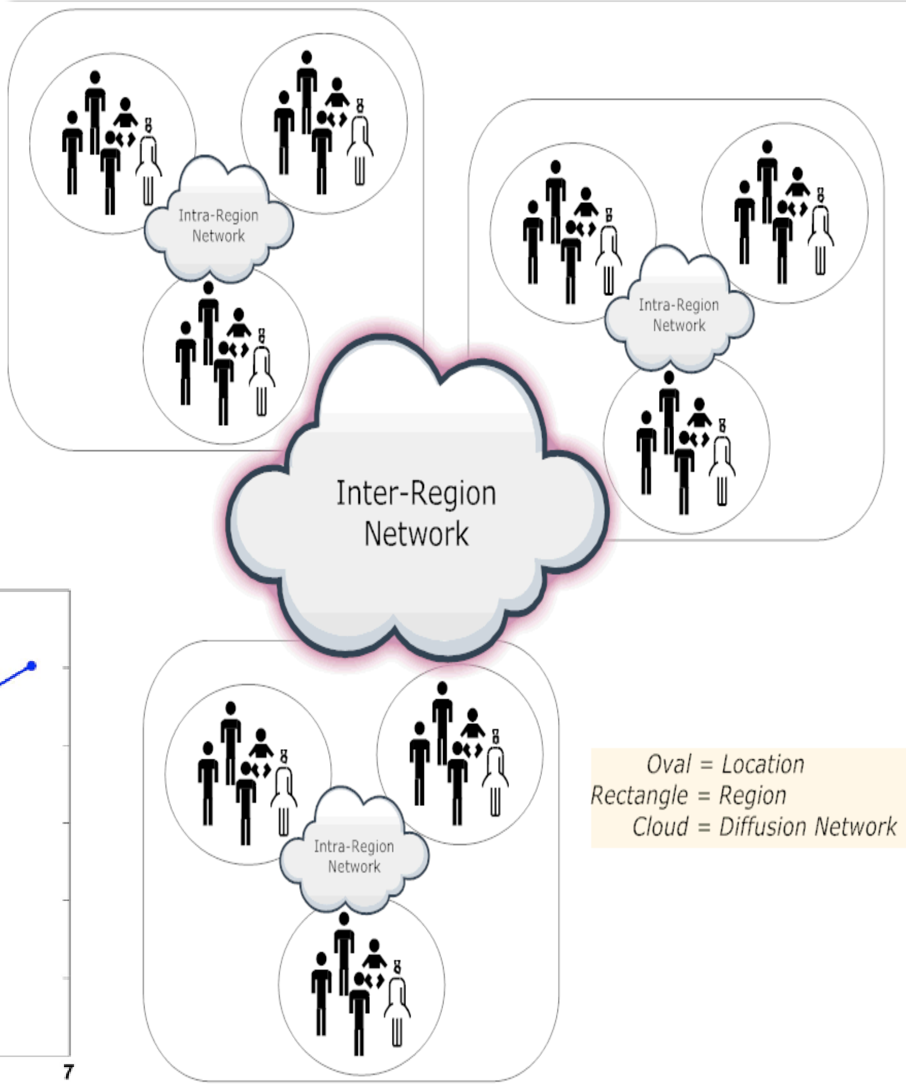


Image from psc.edu

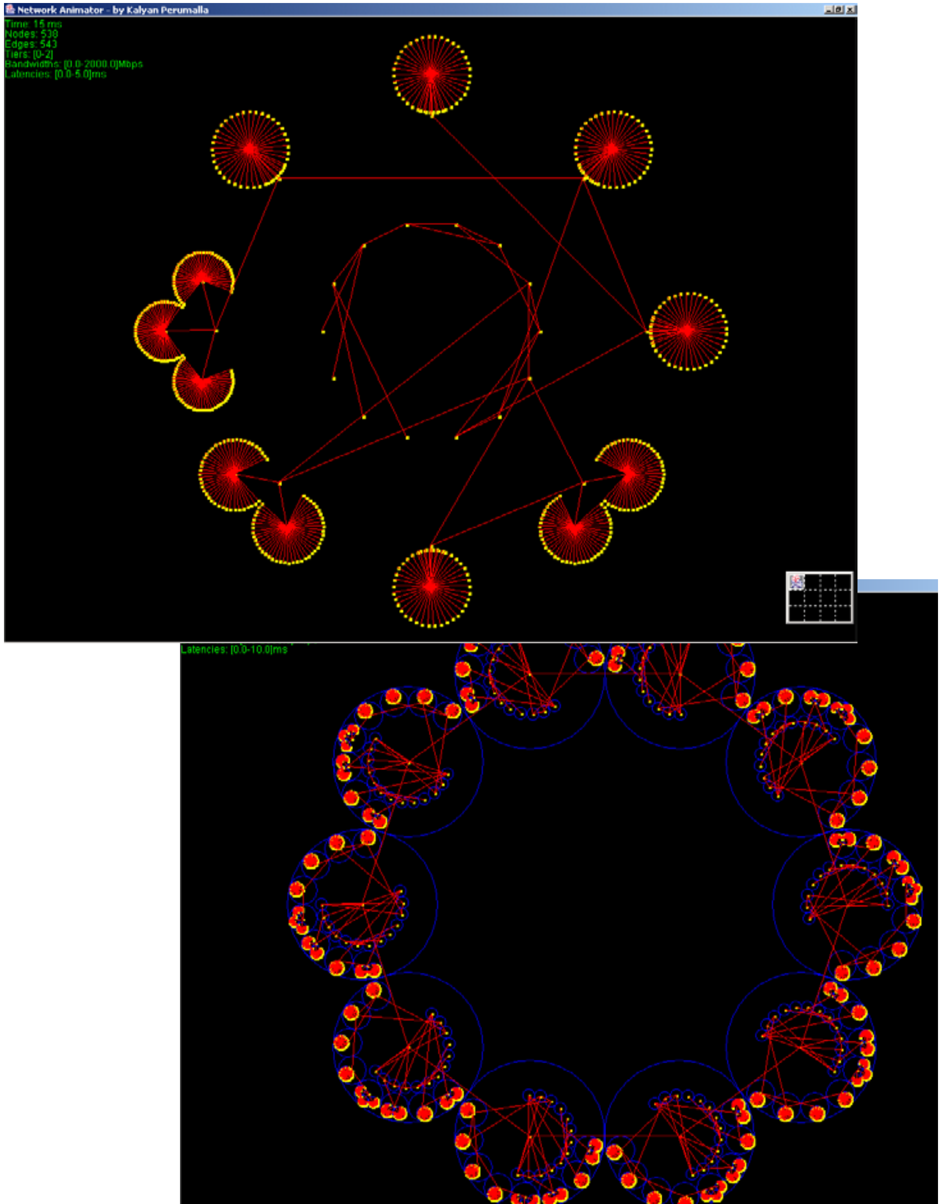
Recent results





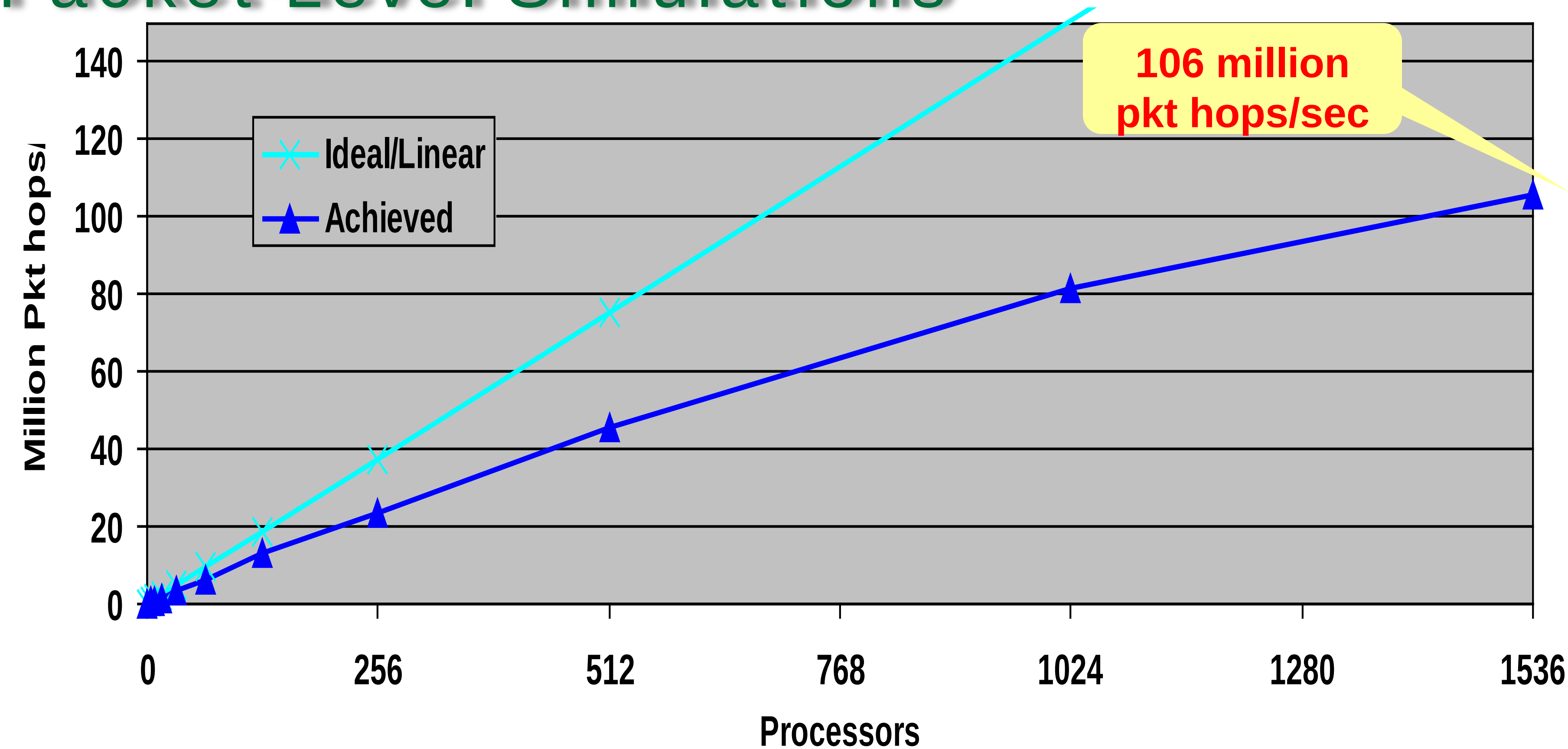


Cyber-infrastructure



- Bandwidth-limited worms
- E.g., Slammer worm of early 2000's
- Throttling and spread are tightly inter-twined

Cyberinfrastructure: Packet-Level Simulations



- Number of packet transmissions simulated per sec
- *Campus network* scenario (500 packets/flow, TCP)
- Scales well to large number of processors, up to 4 million nodes

Summary

- Feedback is a major differentiator
  – Compared to previous models and simulations
- Feedback is a commonality we see in a variety of domains
- In all, computation is dramatically increased

- High Performance Computing seems essential
  – In absence of additional insights into the models
  – Or, alternatively, to gain additional insights into the models