Overview of the Modeling Process 2: Formulation & Beyond

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Using Modeling to Prepare for Changing Healthcare Needs

Duke-NUS

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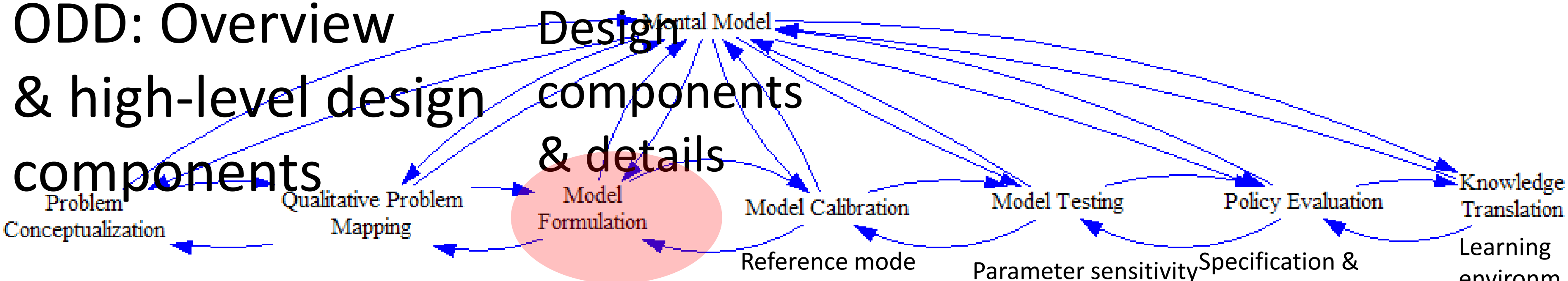
ABM Modeling Process Overview

ODD: Overview & high-level design components

ODD: Design components & details



Problem/research question articulation

Patterns for explanation

Model scope/boundary selection (endogeous, exogenous,ignored)

Key entities & their relationships
- Agents (&collectives)
- Environment
- Nesting hierarchy or network diagrams

Output of interest

State charts
Parameter & state variables
Qualitative State charts
Influence & Causal loop diagrams
Multi-agent interaction diagrams
Process flow structure
Key events
Rough model time & spatial extent
Observers to measure outputs

Specification of
- Parameters
- Quantitative causal relations
- Decision/behavior rules
  - Transitions
- Interactions
  - Messaging &handlers
  - Resources
- Relationship dynamics
- Mobility dynamics
- Initial conditions

Reference mode reproduction

Matching of intermediate time series

Matching of observed data points

Constrain to sensible bounds
Structural sensitivity analysis

Parameter sensitivity analysis

Cross-validation
- Formal
- w/Discovered
  - Patterns

Robustness tests

Extreme value tests

Unit checking

Problem domain tests

Specification & investigation of intervention scenarios
Investigation of hypothetical external conditions

Cross-scenario comparisons (e.g. CEA)

Learning environments (e.g. DISimS)

Visualizations

Model Formulation

- Model formulation elaborates on problem mapping to yield a fully specified, quantitative model
- Key missing ingredients: Specifying unambiguous specification for
    - Statechart transitions
    - Flows (in terms of other variables)
    - Observer processes
    - Intermediate variables
  - Parameter values

Model Specification Mechanisms

Stock & Flow Models: "Hedgehog Knowledge"

- Small modeling vocabulary
- Power lies in combination of a few elements
- Analysis conducted predominantly in terms of elements of model vocabulary

Agent-Based Modeling: "Fox Knowledge"

- Large modeling vocabulary
- Different subsets of vocabulary used for different models
- Power in flexibility & combination of elements
- Variety in analysis focus

ABMs: Larger Model Vocabulary & Needs

- Events
- Multiple mechanisms for describing dynamics
  - State diagrams
  - Stock and flow
  - Custom update code
- Inter-Agent communication (sending & receiving)
- Multiple types of transitions
- Diverse types of agents
- Spatial & topological connectivity & patterning
- Subtyping
- Mobility & movement
- Graphical interfaces
- Data output mechanisms
- Stochastics complicated
  - Scenario result interpretation
  - Calibration
  - Sensitivity analysis
- Synchronous & asynchronous distinction, concurrency

Process Interaction & Scheduling

- In addition to specifying the processes in isolation, try to describe process interaction e.g.
  - A transmission process is not triggered until a person is sexually active
  - All reporting takes place at the very end of the day, and is done before resetting reporting counters
  - All agents first note the status of the agents around them, and only then perform updates to location
- Ask yourself on what other processes a given process depends

Concurrency

- Two or more processes may be operating concurrently (“in parallel”)
  - e.g.: Operation of different agents, agents & reporting processes, graphical interface & model

Dependencies: Synchronous vs. Asynchronous

- Suppose process A depends on information produced by process B
  - e.g. depends on knowing something produced via B
- Synchronous processes: Applied sequentially, so that A must wait for B to proceed (e.g. A calls B)
- Asynchronous processes: No “blocking” (waiting) by A for B (e.g. B sends a message to A)
  - In agent-based modeling, most interactions between agents are considered *asynchronous* => inter-agent communication is accomplished via asynch. messaging

ODD: 3 Broad Components

- Overview: model goals & high level scope & design
- Design concepts: Different aspects of design being considered
- Remaining elements

ODD Design Concepts to Consciously Consider

- Origin & character of basic principles underlying model
- Emergence: To what degree are results pre-programmed vs. arising naturally out of a myriad of interactions
- Adaptation: How does system evolution lead to entity behavior change?
- Sensing: What information do entities retrieve from world?
- Objectives: Any goal seeking behavior? How interacts w/state?
- Learning: How does experience drive change in strategies?
- Prediction: How do entities anticipate the future?
- Interaction: How do entities interact directly & indirectly?
- Stochastics: Character of & motivation for stochastic effects
- Observation: What information & associated processes are required for operational use or for testing & confidence bldg

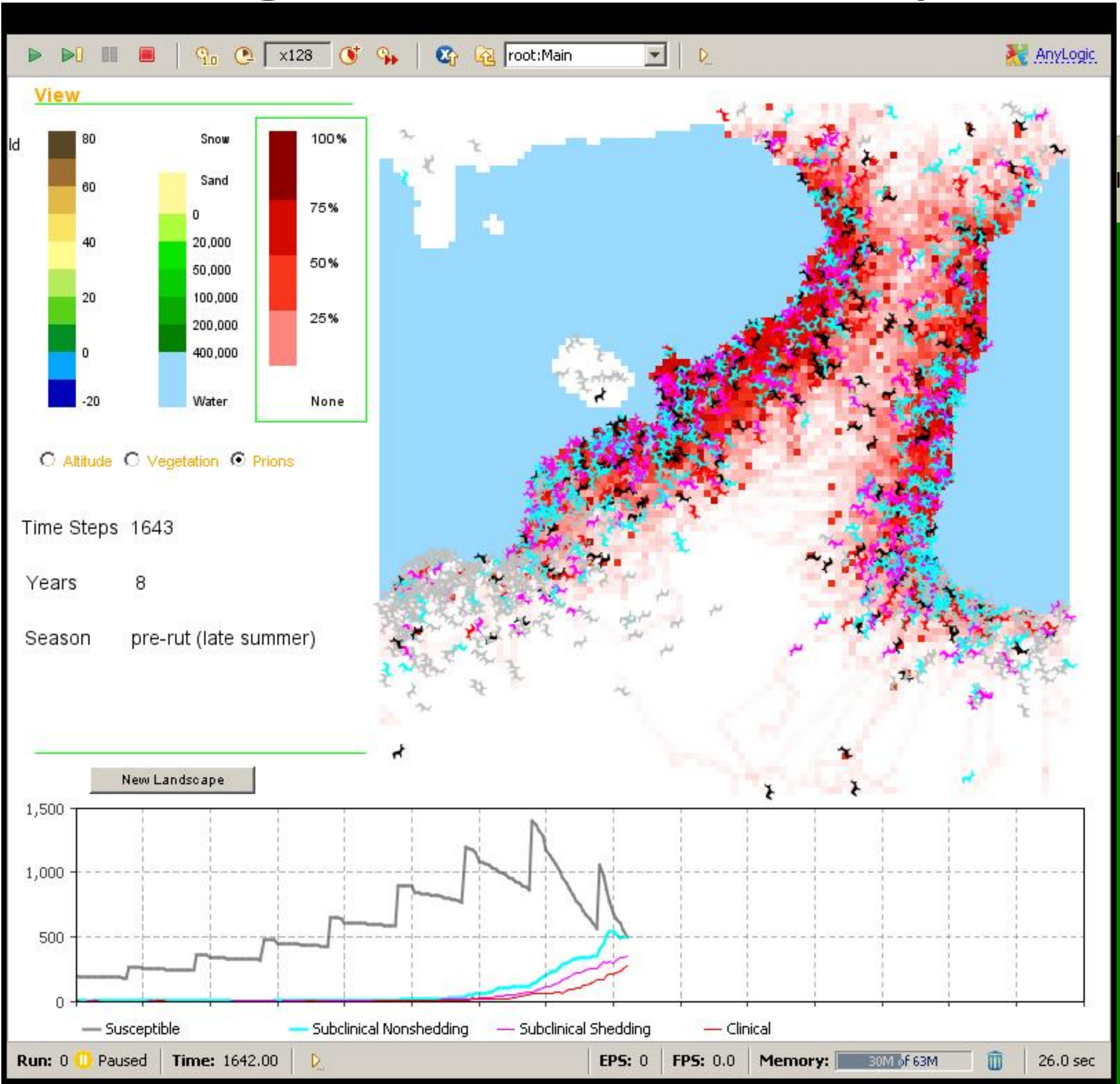
Sensing

- Information sensed from other agents & environments is key to adaptation & decisions
- Need to consider what is sensed
- May want to capture fact that entity perception is
  - Localized (e.g. risk perception, cf decision making with driver's view of road compared to with perfect knowledge of traffic flows across city)
  - Error prone
  - Delayed
  - This can fundamentally alter dynamics: e.g.
    - Instability: Fragility of "Tit for Tat" to misunderstandings
    - Negative feedback: Sensing to correct driving path

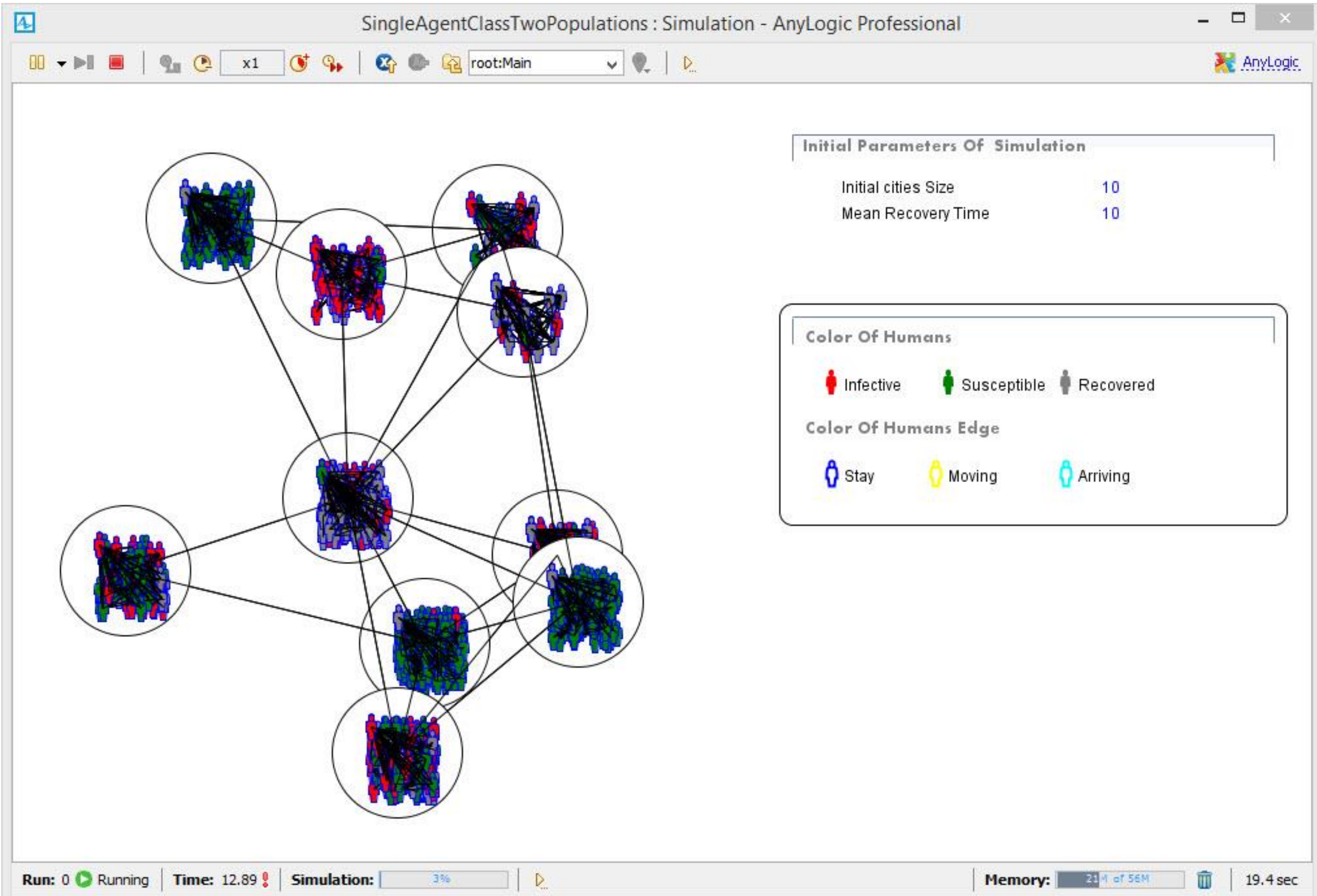
Emergence

- To what degree are the results directly captured by assumptions? (i.e. to what degree are we presupposing what we are trying to demonstrate?)
- One ABM viewpoint: Until we can robustly *generate* a phenomenon, we don’t really understand it
- To what degree to results emerge from complex interaction of other factors where the behavior of interest is never itself described in any way
  - This is ideally what is sought
    - it allows more of a real explanation
    - Permits greater generality (anticipating system behavior under unobserved situations)
  - e.g. waves of infection in spatial SIR model
  - In CWD Model: Clustering of prions along
    - the lakeshore margin
    - High traffic cooridors

Emergent Behavior: Spatial/Geographic



A Multi-Level (Dynamic) Model



Adaptation

- How does agent *behavior* exhibited depend on the
  - Local or global environment
  - Surrounding agents
- To what degree is agent behavior fixed based on predefined rules (just playing out to understand collective effect of rules themselves) vs. potential for emergence associated with inter-agent or agent-environment *behavioral* interaction, which often leads to correspondingly richer emergent behavior
  - Note that can still have inter-agent emergence without adaptation -- e.g. in an infection spread model. But the presence of adaptation means that the feedbacks and emergent phenomena can be that much richer

How Does Behavior Depend on Context?

- We have great flexibility in representing agent rules
- Some agents may be consciously objective seeking
- Just reproducing statistical patterns (likelihood changes in tobacco use over time)
  - Limited generality under counter-factuals
- Examples of ways might depend on context
  - Behavior change due to risk perception
  - Moving to a new neighborhood or hunting/gathering ground
  - Remembering insults and changing strategies (e.g. to defect) with respect to a neighbor in a connection matrix
  - By acquiring new memes or information from a neighbor

Incorporating Observed Patterns: 3 Ways

- Building patterns directly into model (likelihood of state transitions , mixing matrix per observations)
  - e.g. Fraction of time spent in different states (foraging, new lake margin, near grain bins)
  - E.g. fraction of time spends with different groups
- Building functional dependence of actions on external conditions into the model
  - E.g. mixing matrix as a function of a preference matrix and current population demographics
- Calibrating or validating to patterns
  - Making patterns emerge from lower-level "mechanics"/ "physics" of model
    - e.g. Contacts (or contact networks) emerge from myriad close-proximity spatial interactions between mobile individuals

Observed Patterns as Emergent

- Ideally, we seek to make patterns emerge from lower-level “mechanics”/ “physics” of model
  - e.g. seasonal herd size emerging naturally from grouping rules in CWD model
- With *adaptation*, particularly focusing on dependence of behavioral patterns of an individual on context
  - How do varying circumstances change agent behavior?

Example of Observed Patterns as Emerging from Low-Level Interactions

- Lower food availability => Higher amount of time spent searching for food
- Higher prevalence of Gonorrhea among acquaintances => greater adherence to safer sex practices
- Higher reports of H1N1 infection or vaccination among social contacts => higher chance of getting vaccinated
- Higher risks from diabetes over age as emerging naturally from cumulative damage by glycosylation, etc.
- Greater smoking-related health complaints & sickness in peers with age => Greater likelihood of quitting with age
- Progression of substance abuse caused by underlying organic processes
- Longer infectious period, greater infection severity (peak viremia level), greater transmissibility for individuals with impaired immune functioning emerging from immune repr.
- Higher temperature => greater water seeking

One Kind of Adaptation: Objective Seeking Behavior

- Here, an entity's behavior will depend on trying to maximize some satisfaction criteria
  - Examples of measures: Profit, Utility
  - Example application: Vehicle simulators using where driving behavior depends on consideration of perceived tradeoffs ($, time, familiarity, etc.) of different routes
- How does this vary based on agent's state (e.g. access to resources) or environments
- Bounded rationality: For individuals, strong literature suggests that many decisions are based instead on heuristics

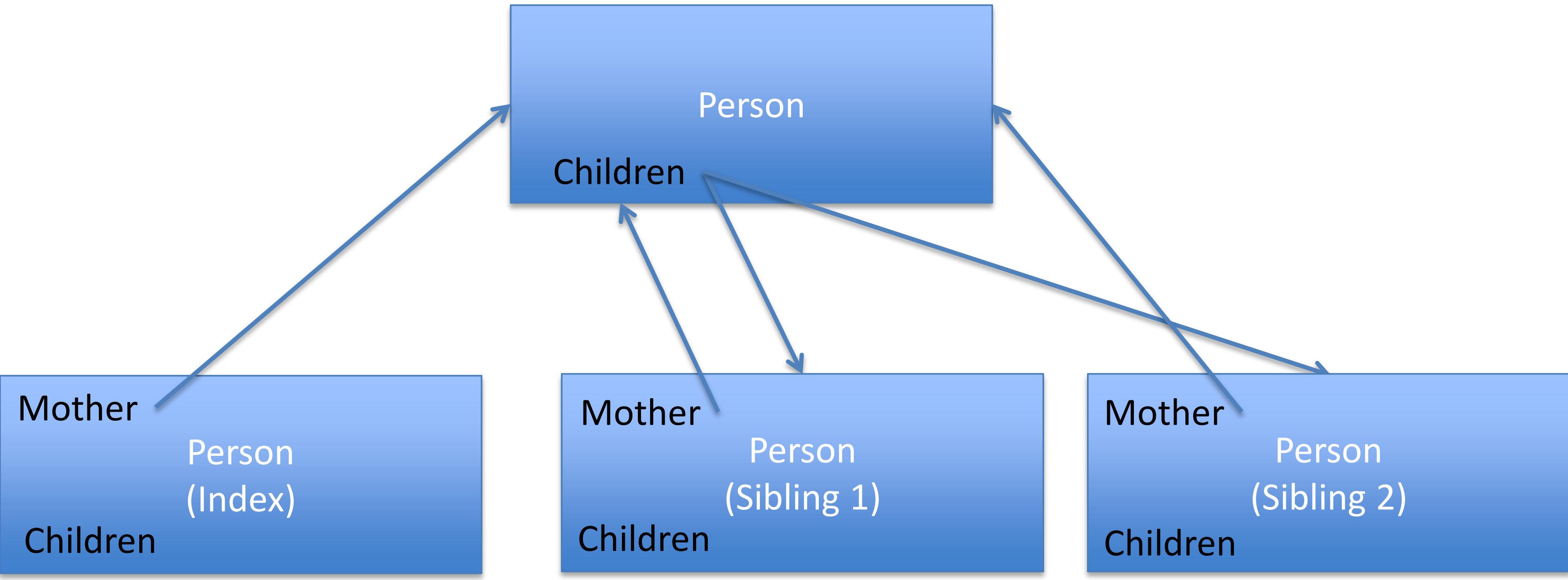
Learning: Changing Adaptive Behavioral Rules Based on Experience

- ABMs can support arbitrarily rich learning that may change adaptive behavior
  - Learning from experience in particular healthcare facilities
  - Trust of different parties based on
    - Direct: Treatment received
    - Indirect: Consistency of observations with claims of other party
- In some cases, this is performed using genetic programming (rules mutate and evolve)
- As a longitudinal phenomenon -- one that involves history -- support of learning & memory is a key advantage offered by ABM

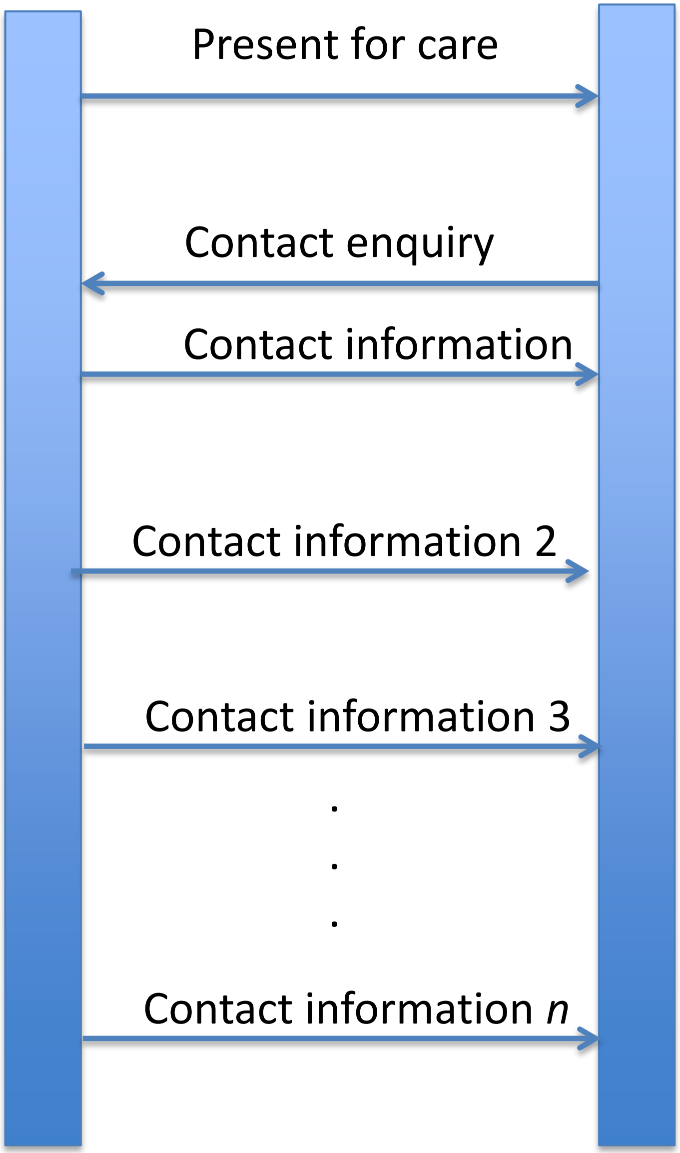
Interaction

- Interaction among entities
  - Agent-agent
  - Agent-environment
- Forms
  - Direct: Agents directly interact with neighbors (e.g. via needle sharing or sexual contact)
  - Indirect: e.g. Via shared resource (depletion of vegetation for browsing by other deer, deposit of droplets with shedded pathogen on surface, or air), via risk perception
- How mediated by space & time? (e.g. transmission range of pathogen, seasonal contact dependence?)

Object Diagram



UML Sequence Diagram



Collectives

- Groupings are a common multi-scale feature
  - Herd, Family, Class, Office
- More than the sum of the parts:
  - Can have significant impact on agent perception or behavior
  - Agent may relocate to join new collective
- Common possibilities
  - Purely emergent phenomenon (e.g. herds in CWD example model): Not reified as agent
    - Sometimes epiphenomenal – no influence, but instead something that can be used for understanding & analysis
    - Sometimes has very material impact on system behavior
  - Reification as agent (e.g. hierarchical SIR model, gang)
    - Collective can then have own processes & state (e.g. history)

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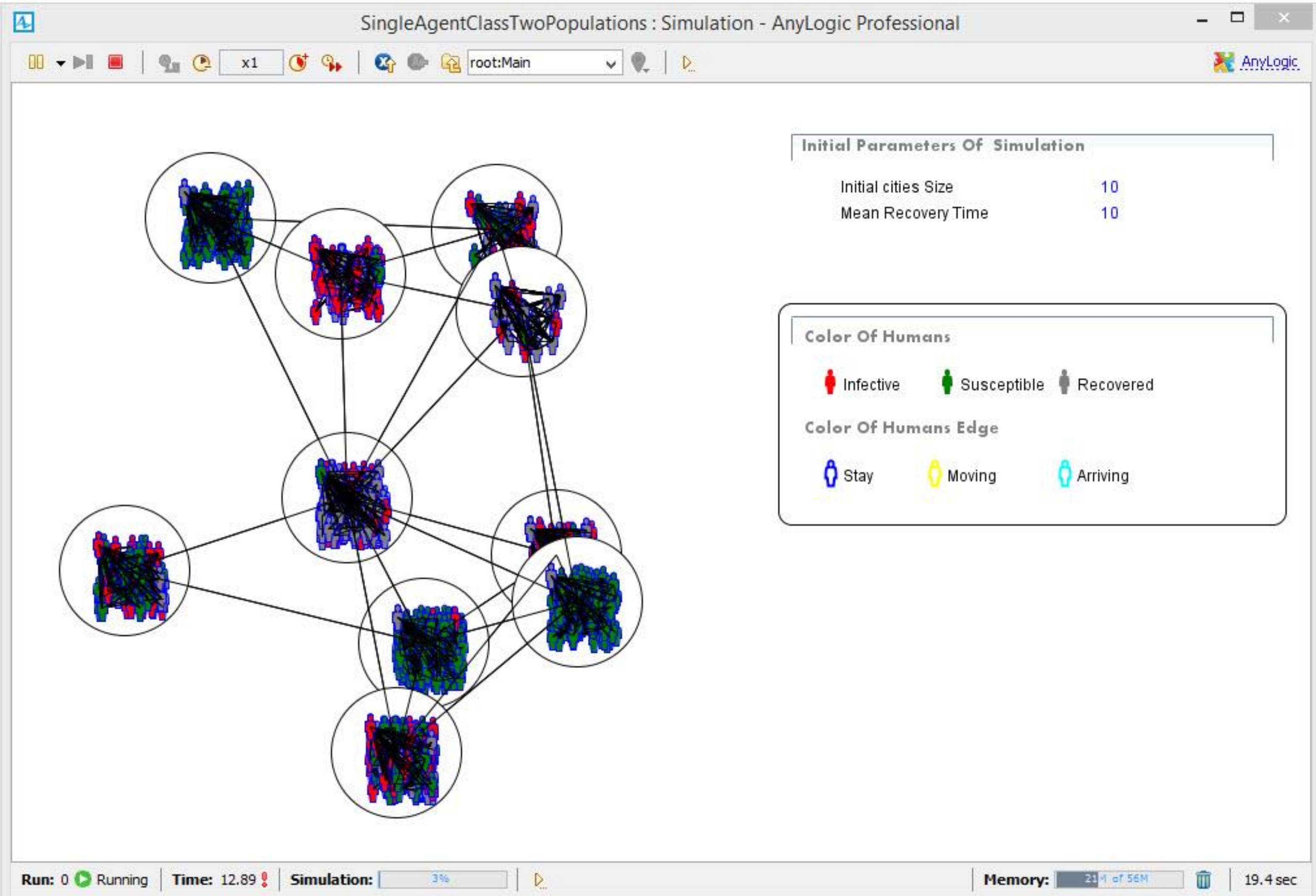


Observer Processes

- With an agent-based model, it is often key to have access to many “views” of the model in operation
  - These can aid in validation (calibration, confidence building) and verification (testing), interpretation, results
- The data collected by such observers is typically epiphenomenal – it does not influence the model
- Often there is a significant amount of mechanism & computational effort involved in realizing these
- Detail complexity: significant investment is often further made in visualization interfaces

ODD: 3 Broad Components

- Overview: model goals & high level scope & design
- Design concepts: Different aspects of design being considered
- Details (Remaining elements)

ODD: Remaining Elements

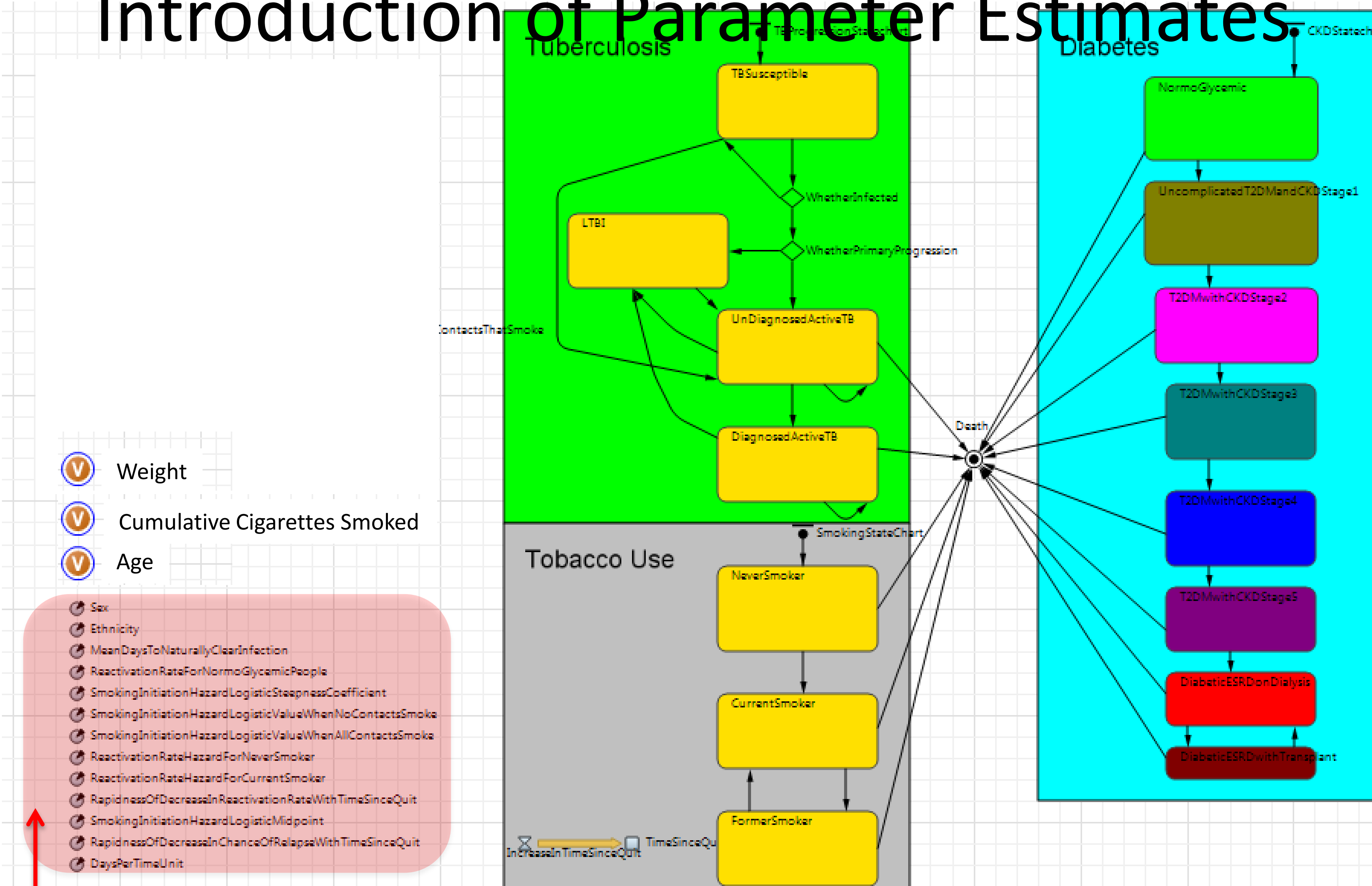
- Initialization
  - Where does initial state come from? Are seeking to make independent of initial state? To test significance of initial state?
- Input data
  - Time series used for model (I think best put in entitiy specification)
- Submodels: Useful abstractions
  - Helpful todescribe early on with broad abstractions (e.g. “partner change”, “go to drink”, “find food”, “stay near mother”
    - Full specification of these are delegated to submodels
  - Seeking low coupling, high cohesion

Sources for Parameter Estimates

- Surveillance data
- Controlled trials
- Outbreak data
- Clinical reports data
- Intervention outcomes studies
- Calibration to historic data
- Expert judgement
- Systematic reviews

Parameter*	Description	Baseline value (units)	Reference
μ	Entry/exit of sexual activity	0.0056 (years^{-1})	Garnett and Bowden, 2000
c	Partner change rate per Susceptible	16.08 (years^{-1})	Approximated from Garnett and Bowden, 2000
β	Probability of infection per sexual contact	0.70	Garnett and Bowden, 2000
φ	Fraction of Infectives who are symptomatic	0.20	Garnett and Bowden, 2000
$1/\gamma$	Latent period	0.038 (years)	Brunham et. al., 2005
$1/\sigma$	Duration of infection	0.25 (years)	Brunham et. al., 2005
θ	Asymptomatic recovery coefficient	1.5	Garnett and Bowden, 2000
$1/\pi$	Duration of naturally-acquired immunity	1 (year)	Approximated from Brunham et. al., 2005

Introduction of Parameter Estimates



These parameters must have constants specified

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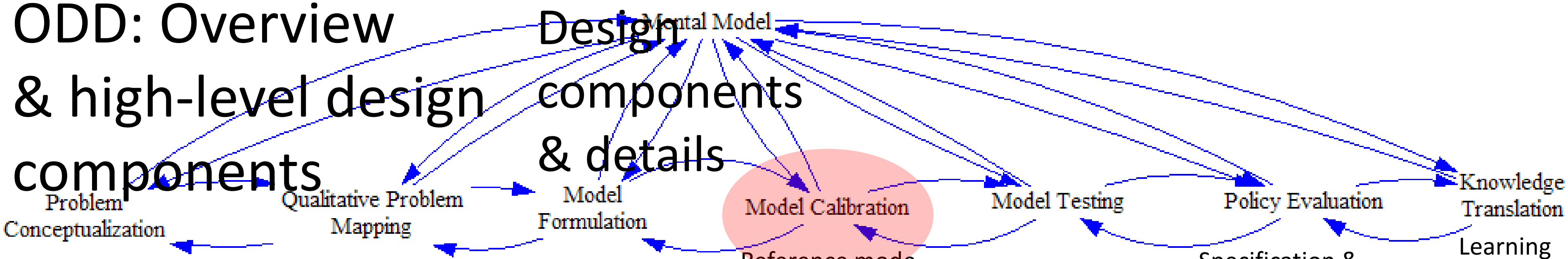

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Visualizations

Calibration

- Often we don't have reliable information on *some* parameters
  - Some parameters may not even be observable!
- Some parameters may implicitly capture a large set of factors not explicitly represented in model
- Often we will calibrate less well known parameters to match observed data
  - "Analytic triangulation": Often try to match against *many* time series or pieces of data at once
- Sometimes we learn from this that our model structure just can't produce the patterns!

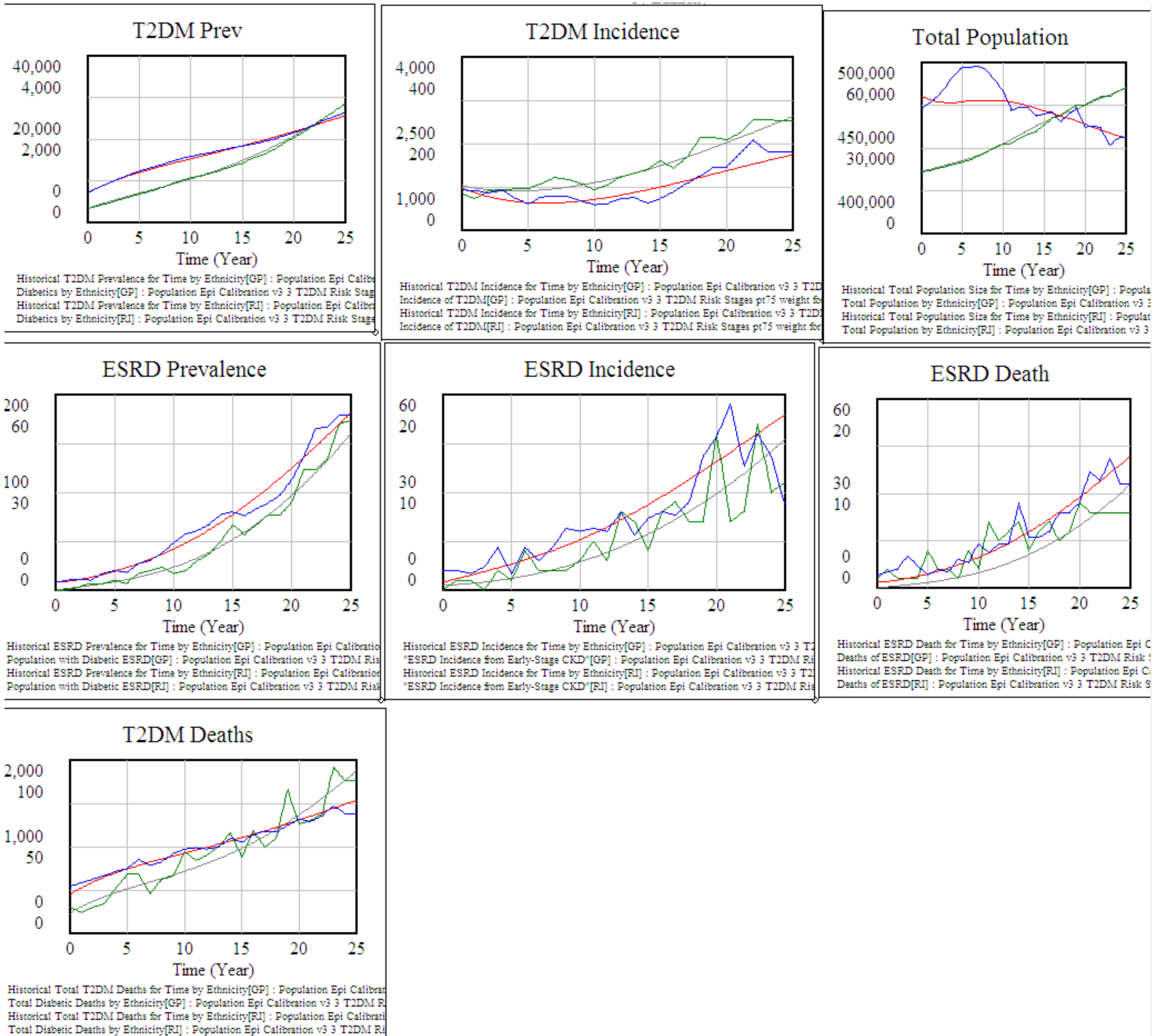
Calibration: “Triangulating” from Diverse Data Sources

- Calibration involves “tuning” values of less well known parameters to best match observed data
  - Often try to match against *many* time series or pieces of data at once
  - Idea is trying to get the software to answer the question: “What must these (less known) parameters be in order to explain all these different sources of data I see”
- Observed data can correspond to complex combination of model variables, and exhibit “emergence”
- Frequently we learn from this that our model structure just can’t produce the patterns!

Calibration

- Calibration helps us find a reasonable (specifics for) "dynamic hypothesis" that explains the observed data
  - Not necessarily the truth, but probably a reasonably good guess – at the least, a consistent guess
- Calibration helps us leverage the large amounts of diffuse information we may have at our disposal, but which cannot be used to directly parameterize the model
- Calibration helps us falsify models

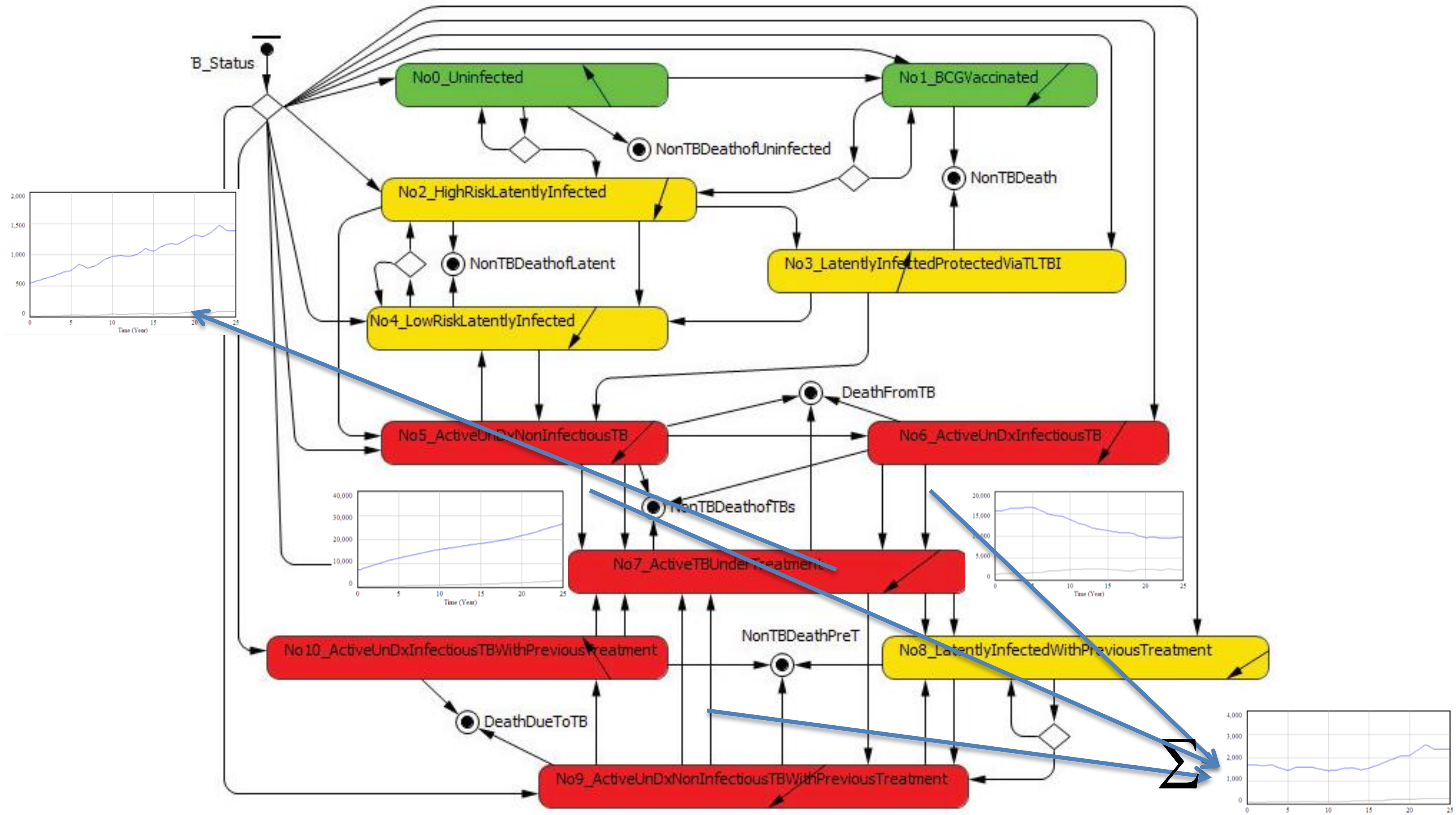
Single Model Matches Many Data Sources



The Pieces of the Elephant

Example Model of Underlying Process&Time Series it Must Match

Here, we are totalling up across the population

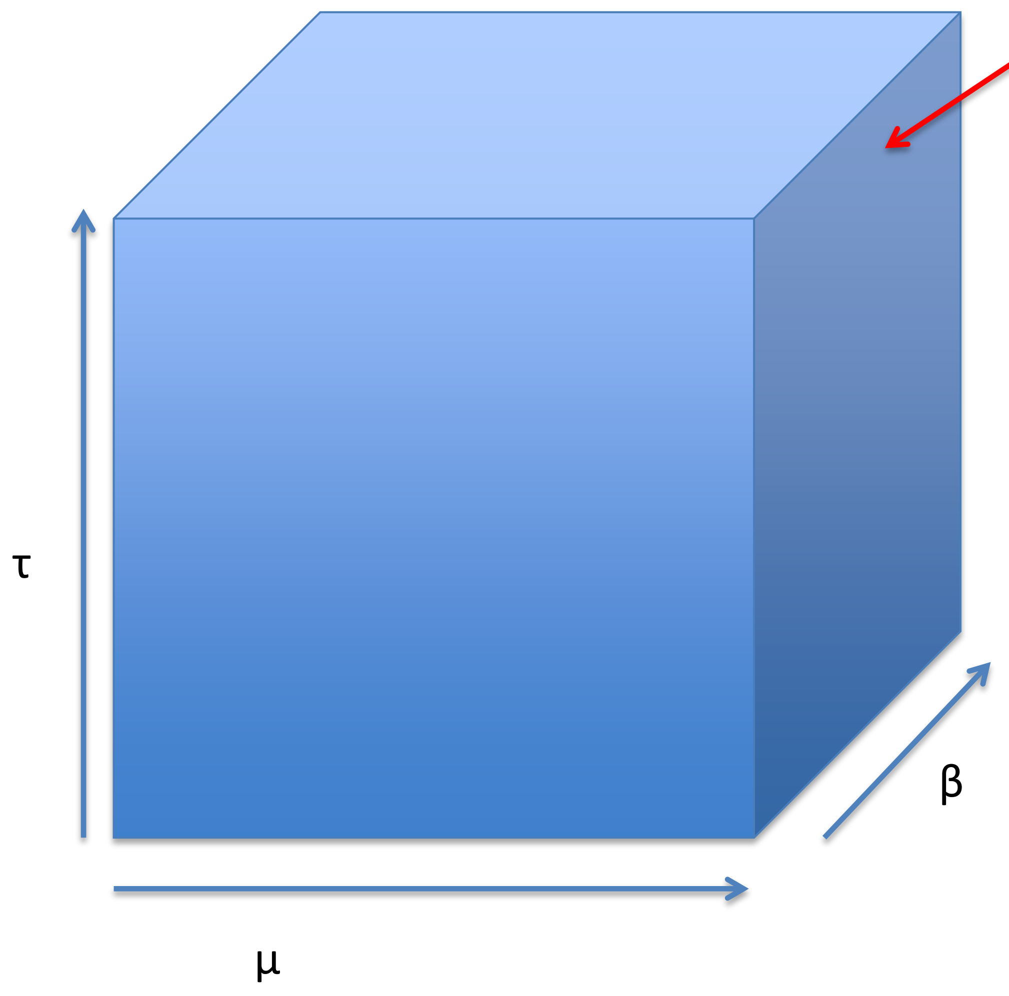


Required Information for Calibration

- Specification of what to match (and how much to care about each attempted match)
  - Involves an "error function" ("penalty function", "energy function") that specifies "how far off we are" for a given run (how good the fit is)
  - Alternative: specify "payoff function" ("objective function")
- A statement of what parameters to vary, and over what range to vary them (the "parameter space")
- Characteristics of desired tuning algorithm
  - Single starting point of search?

Envisioning "Parameter Space"

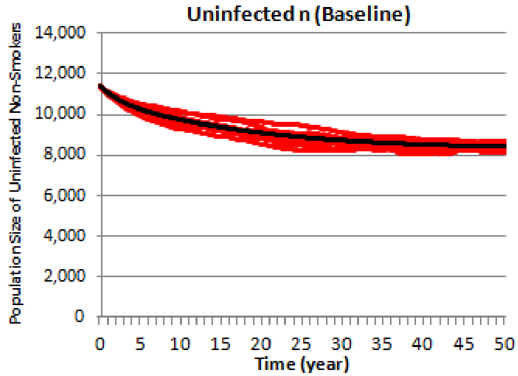
For each point in this space, there will be a certain "goodness of fit" of the model to the collective data

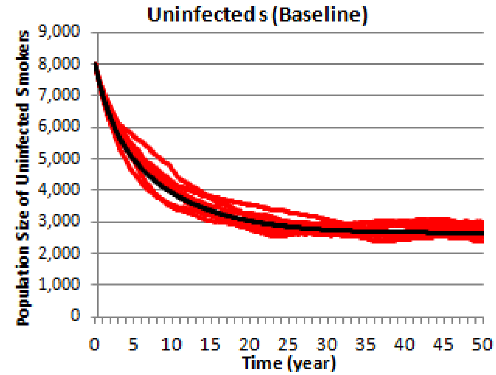


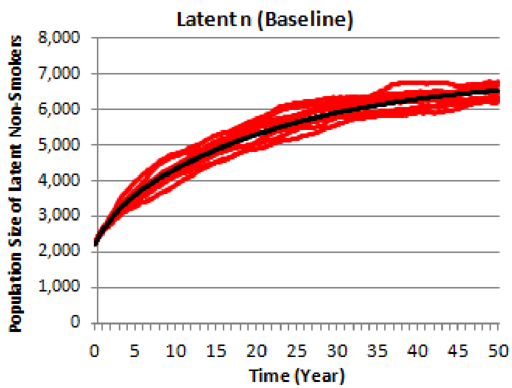
Stochastics in Agent-Based Models

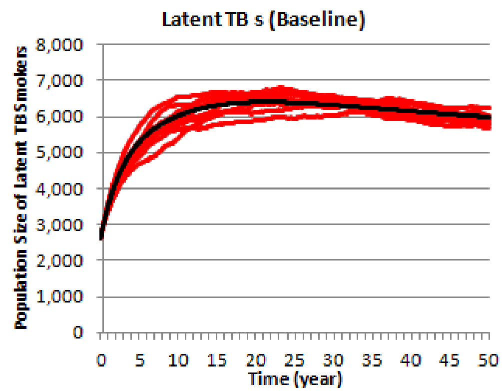
- Recall that ABMs typically exhibit significant stochastics
  - Event timing within & outside of agents
  - Inter-agent interactions
- Can have a pronounced impact on system evolution
- Such stochastics can account for observed patterns that are otherwise hard to explain
- When calibrating an ABM, we wish to avoid attributing a good match to a particular set of parameter values simply due to chance
- To reliably assess fit of a given set of parameters, we need to repeatedly run model realizations
  - We can take the mean fit of these realizations
- Often best to match not time series, but summaries

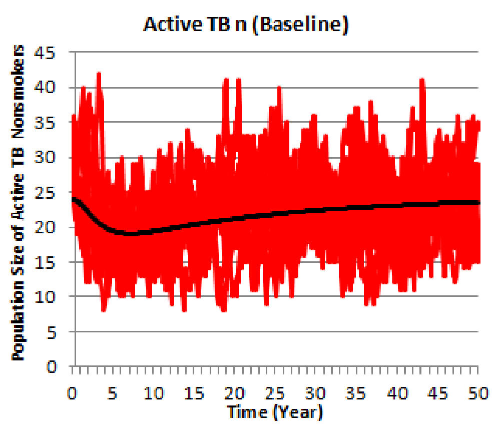
Examples of Stochastics (Compared to Mean Field Deterministic Model)

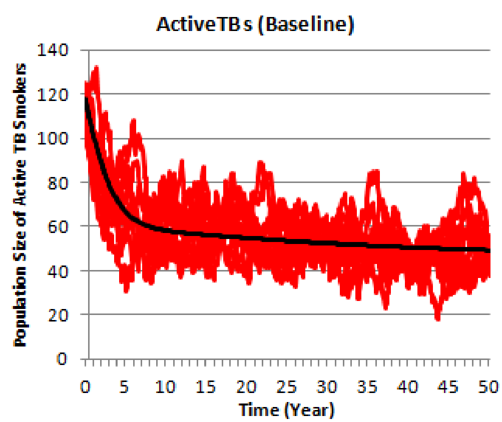




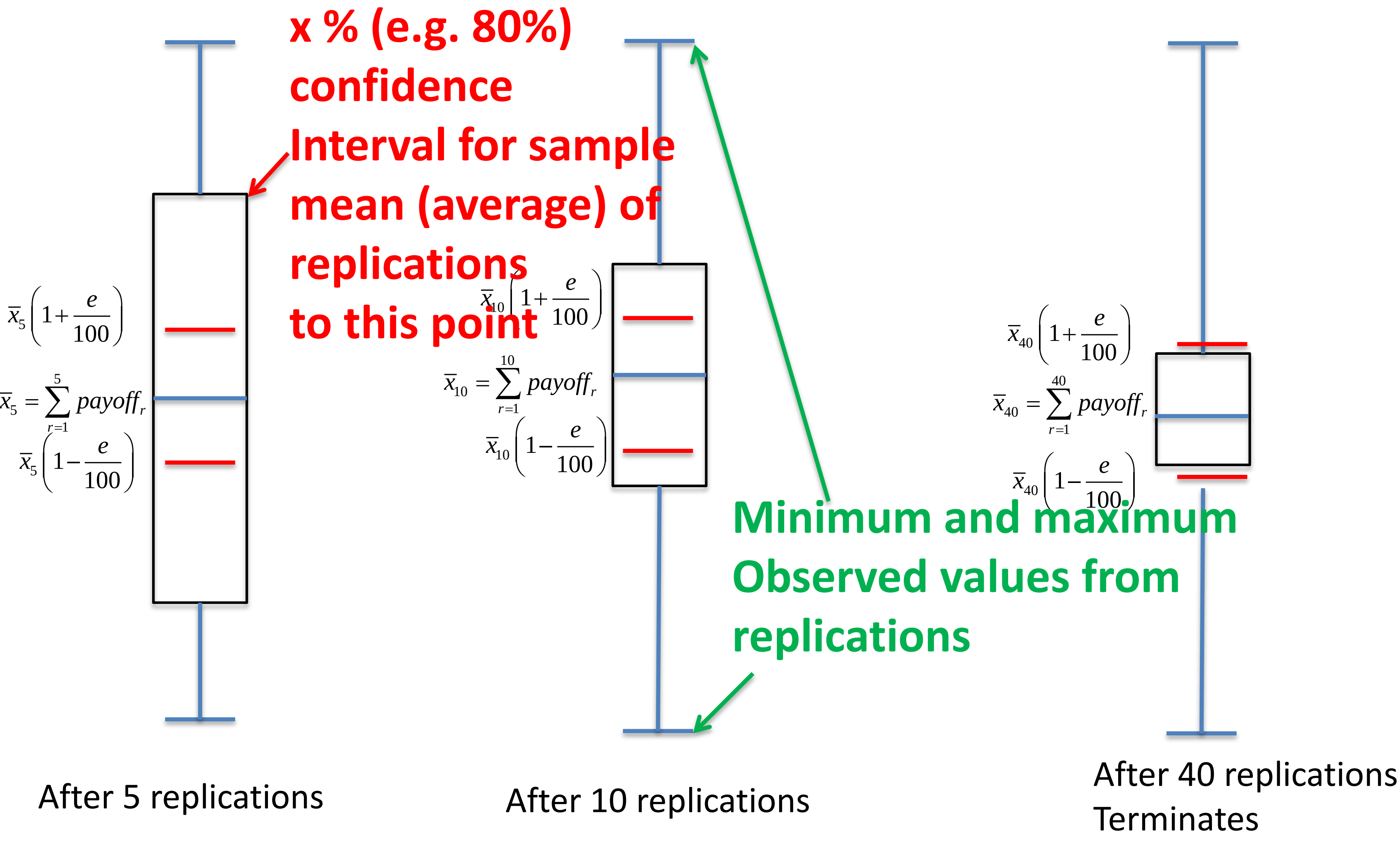








Example


x % (e.g. 80%) confidence
Interval for sample mean (average) of replications to this point
$\bar{x}_5\left(1+\frac{e}{100}\right)$
$\bar{x}_5=\sum_{r=1}^{5} payoff_r$
$\bar{x}_5\left(1-\frac{e}{100}\right)$
$\bar{x}_{10}\left(1+\frac{e}{100}\right)$
$\bar{x}_{10}=\sum_{r=1}^{10} payoff_r$
$\bar{x}_{10}\left(1-\frac{e}{100}\right)$
$\bar{x}_{40}\left(1+\frac{e}{100}\right)$
$\bar{x}_{40}=\sum_{r=1}^{40} payoff_r$
$\bar{x}_{40}\left(1-\frac{e}{100}\right)$
Minimum and maximum Observed values from replications
After 5 replications
After 10 replications
After 40 replications
Terminates

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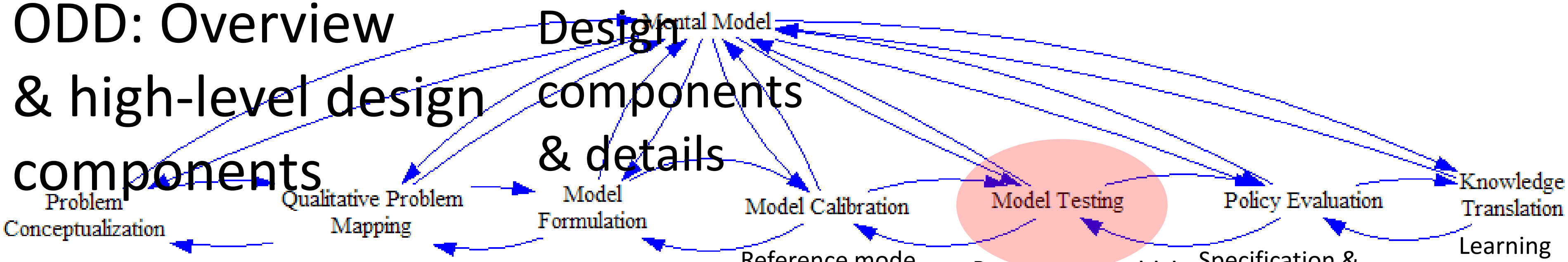

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Visualizations

Units & Dimensions

- Distance
  - Dimension: Length
  - Units: Meters/Fathoms/Li/Parsecs
- Frequency (Growth Rate, etc.)
  - Dimension:1/Time
  - Units: 1/Year, 1/sec, etc.
- Fractions
  - Dimension: “Dimensionless” (“Unit”, 1)
  - Units: 1

Dimensional Analysis

- DA exploits structure of dimensional quantities to facilitate insight into the external world
- Uses
  - Cross-checking dimensional homogeneity of model
  - Deducing form of conjectured relationship
    (including showing independence of particular factors)
  - Sanity check on validation of closed-form model analysis
  - Checks on simulation results
  - Derivation of scaling laws

  * Construction of scale models
  - Reducing dimensionality of model calibration, parameter estimation

Uncertainty Analyses

- Same relative or absolute uncertainty in different parameters may have hugely different effect on outcomes or decisions
- Help identify parameters that strongly affect
  - Key model results
  - Choice between policies
- We place more emphasis in parameter estimation into parameters exhibiting high sensitivity

Uncertainty Analysis: Initial Value

- Frequently we don’t know the exact state of the system at a certain point in time
- A very useful type of sensitivity analysis is to vary the initial value of model stocks
- In Vensim, this can be accomplished by
  - Indicating a parameter name within the “initial value” area for a stock
  - Varying the parameter value

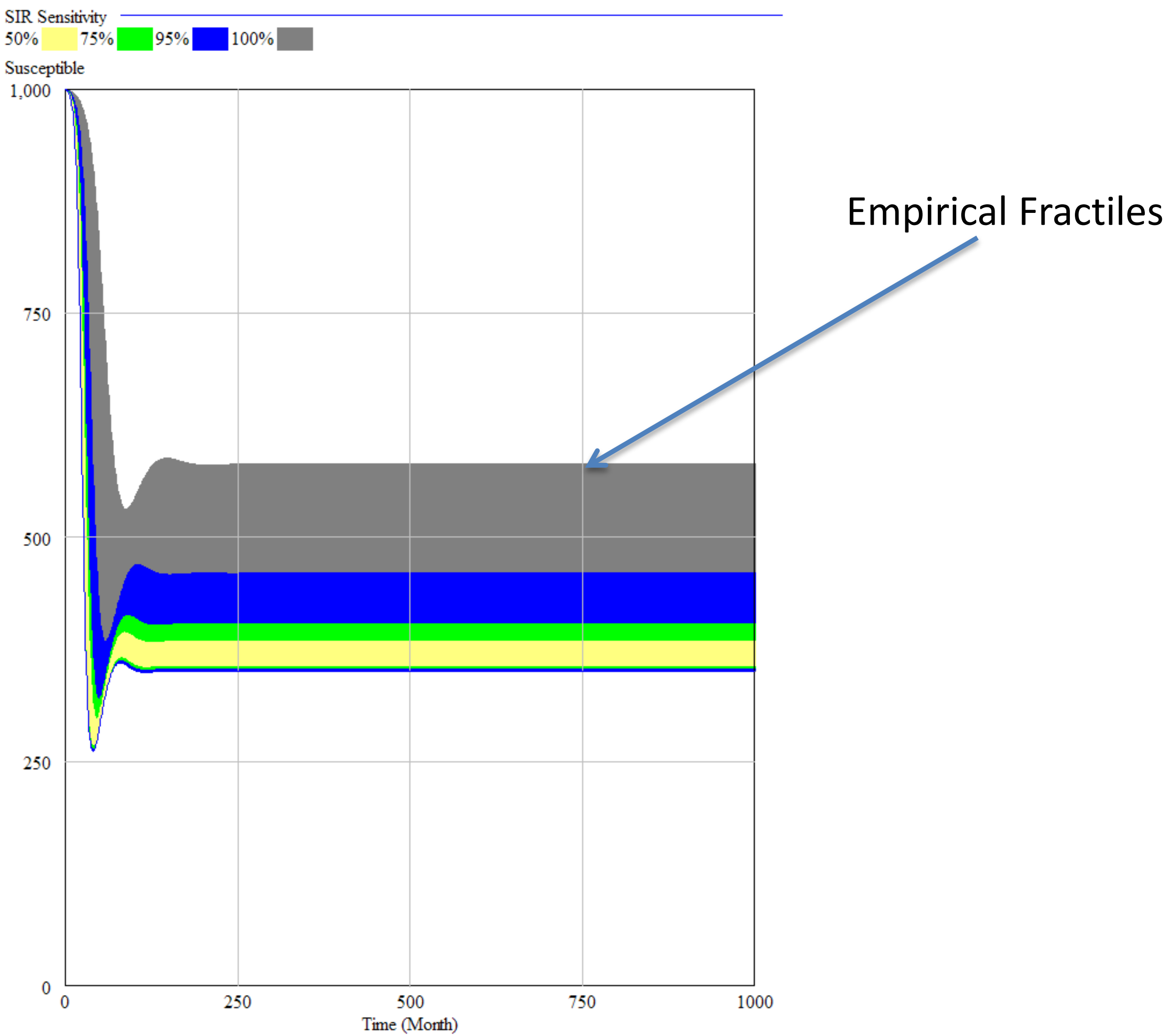
Robustness Analysis

- To what degree are model conclusions robust under changing model structural and other large assumptions?
  - Distinguish cases where
    - Results depends on something essential about the model
    - Results depend on happenstance of simplifying assumptions
      - e.g. spatial neighborhood assumption, size or granularity of space, convenient assumptions regarding rules or what is known
- We want to rule out cases where getting “right result for wrong reasons”!
- Seek to find whether conclusions change radically when just a few assumptions are changed?
- Process is similar to what used for submodel testing, but done for entire model

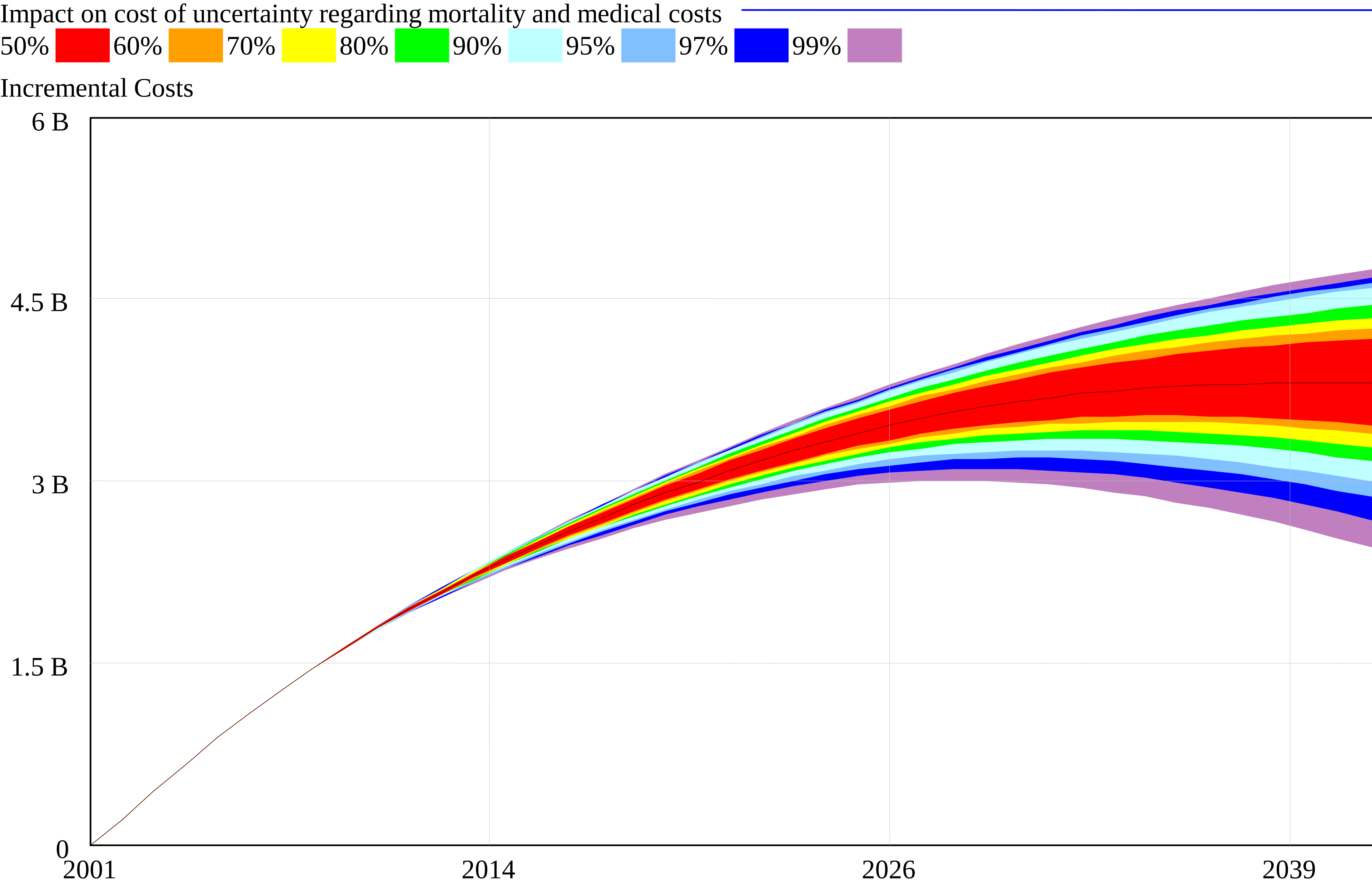
Imposing a Probability Distribution Monte Carlo Analysis

- We feed in probability distributions to reflect our uncertainty about one or more parameters
- The model is run many, many times (realizations)
  - For each realization, the model uses a different draw from those probability distribution
- What emerges is resulting probability distribution for model outputs

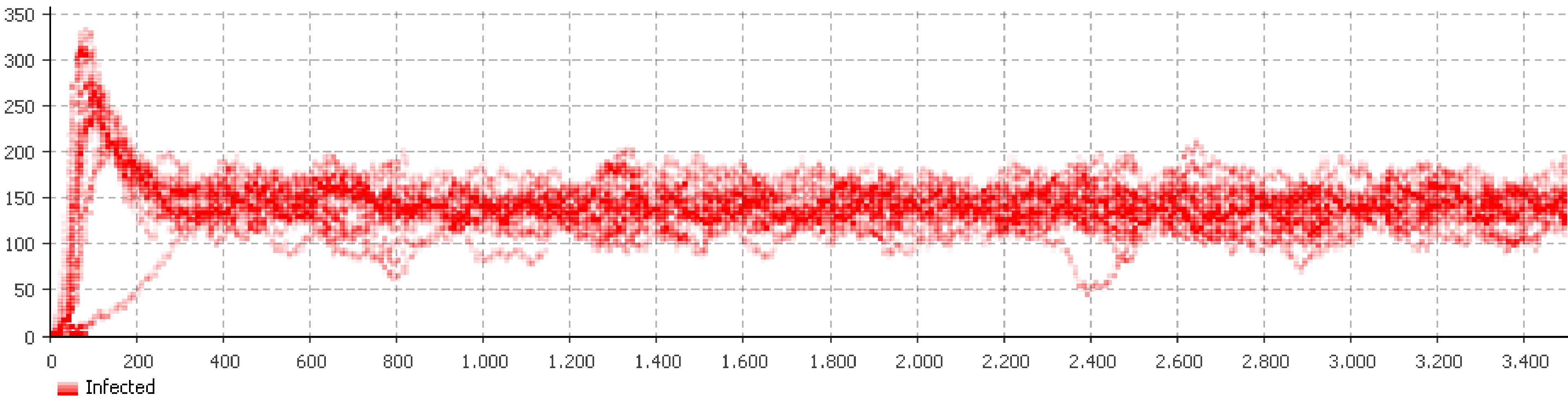
Example Resulting Distribution



Static Uncertainty

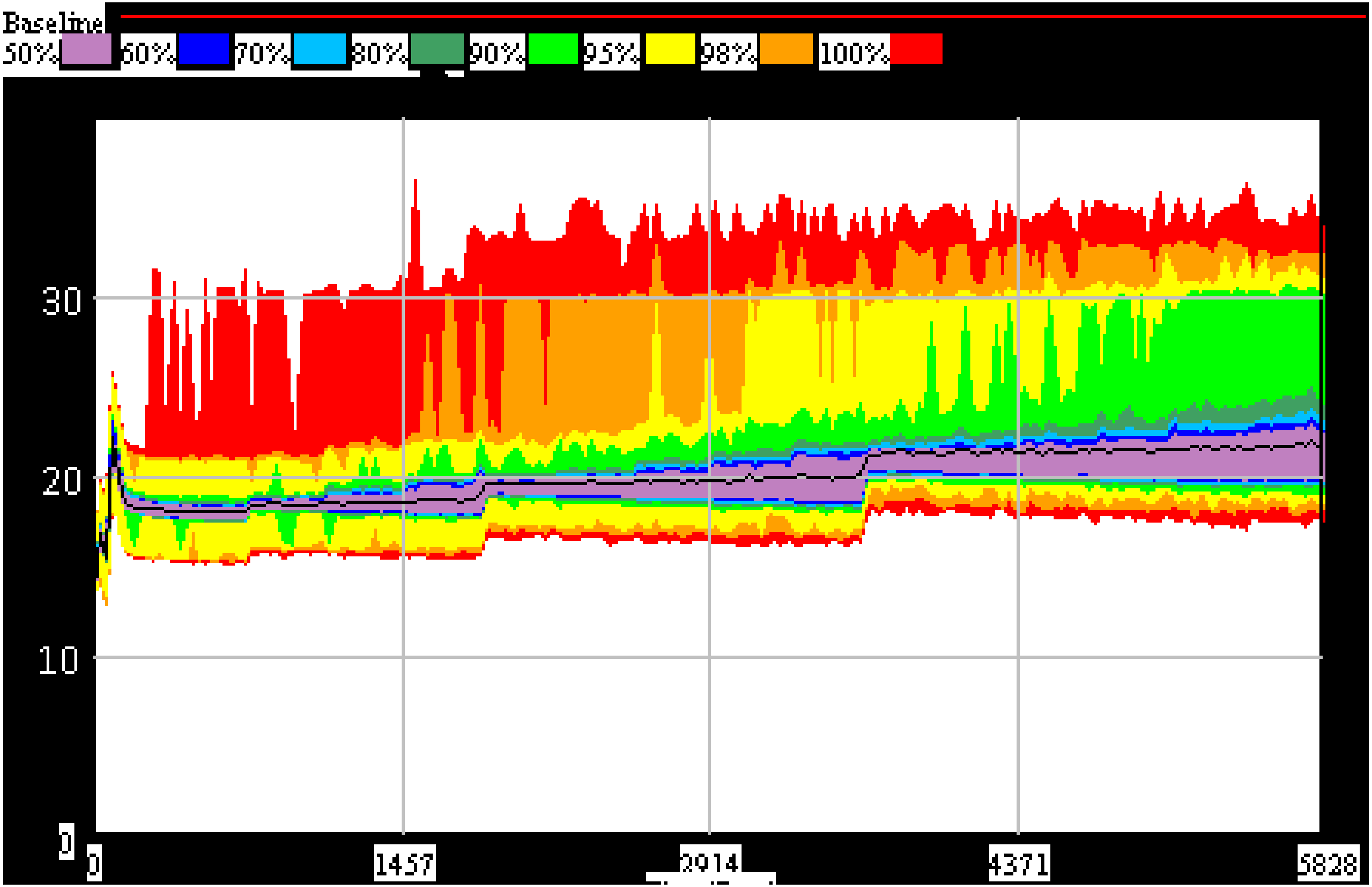


Dynamic Uncertainty: Stochastic Processes



This is a form of sensitivity analysis, but because we are capturing effects of model stochastics – rather than our lack of knowledge, we don't term "uncertainty analysis"

Dynamic Uncertainty: Stochastic Processes



Mathematical Analysis of Models

System Linearization (Jacobian)

$$\begin{bmatrix} -\beta\, Infectives - \delta & -\beta\, S - \delta \\ \beta\, Infectives & \beta\, S - \dfrac{1}{\mu + \dfrac{\tau\, Infectives}{h}} + \dfrac{Infectives\, \tau}{\left(\mu + \dfrac{\tau\, Infectives}{h}\right)^2 h} \end{bmatrix}$$

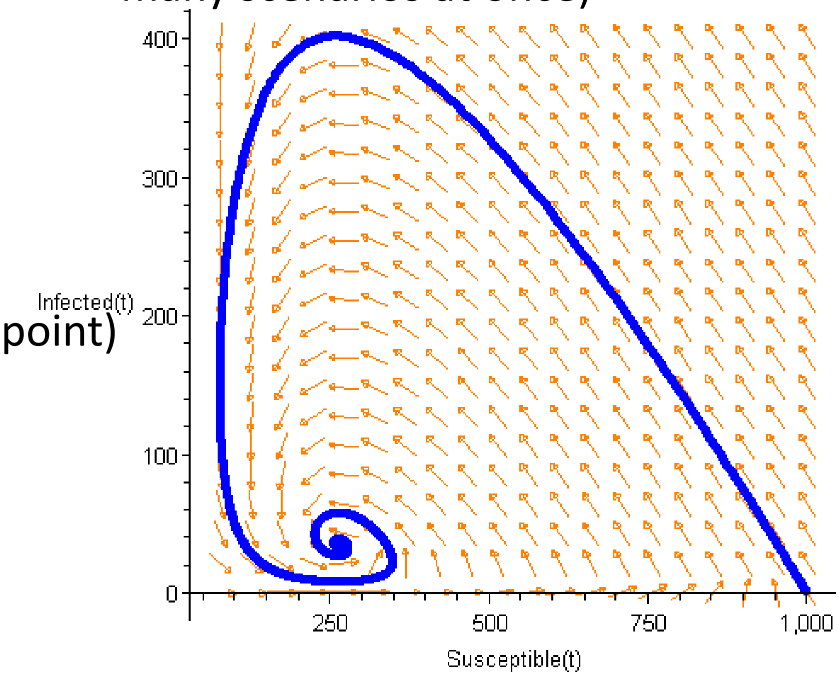
Fixed-Point Criteria

$$\dot{S} = -c\left(\frac{I}{N}\right)\hat{\beta} S + R\delta = 0$$

$$\dot{I} = c\left(\frac{I}{N}\right)\hat{\beta} S - \frac{I}{\mu + \tau \dfrac{I}{h}} = 0$$

$$\dot{R} = \frac{I}{\mu + \tau \dfrac{I}{h}} - R\delta = 0$$

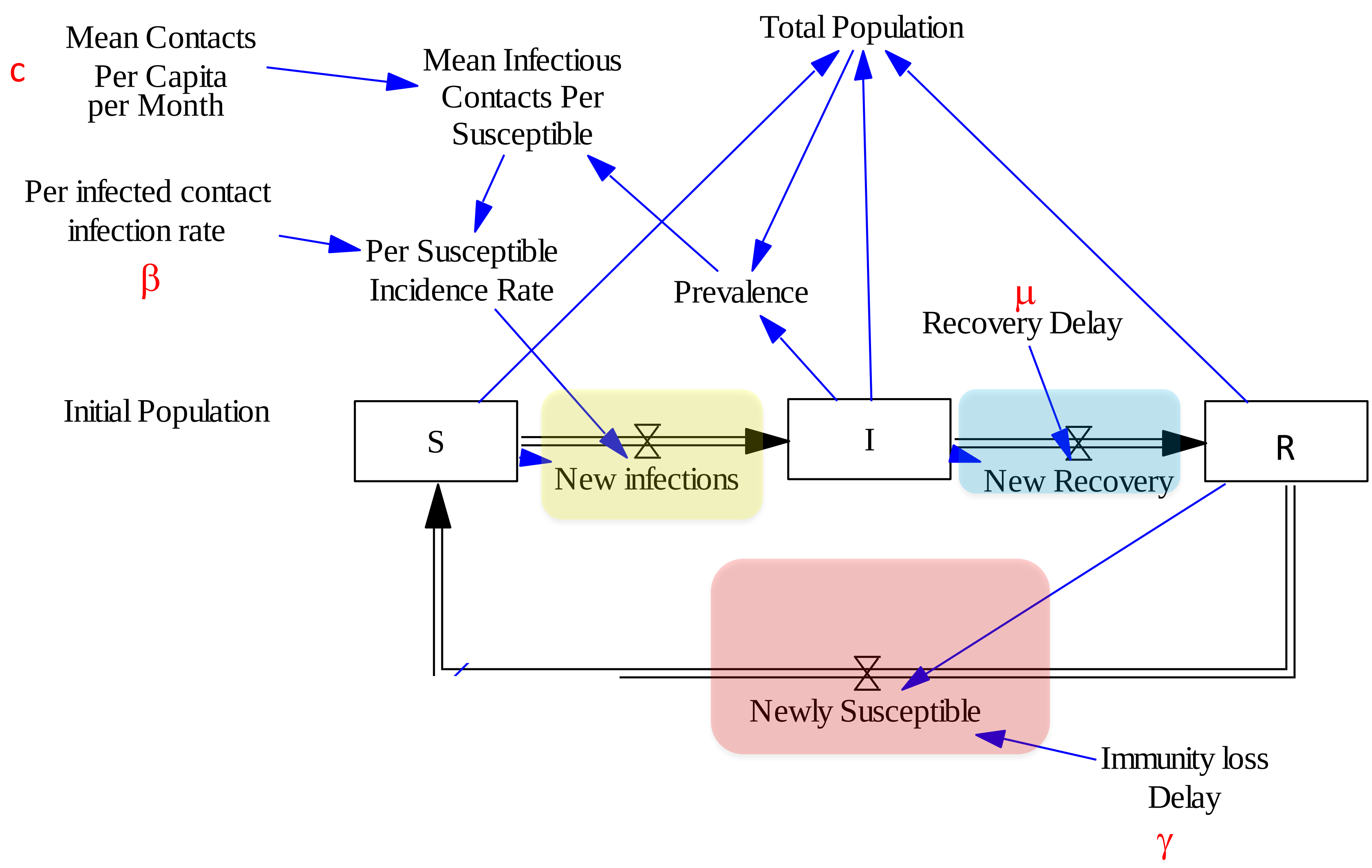
State space diagram (reasoning about many scenarios at once)



Eigenvalues (e.g. for stability analysis around fixed-point)

$$\frac{1}{2}\beta S - \frac{1}{2}\frac{1}{\mu + \frac{\tau\, Infectives}{h}} + \frac{1}{2}\frac{Infectives\, \tau}{\left(\mu + \frac{\tau\, Infectives}{h}\right)^2 h} - \frac{1}{2}\beta\, Infectives - \frac{1}{2}\delta$$
$$+ \frac{1}{2}\left(\left(\beta S - \frac{1}{\mu + \frac{\tau\, Infectives}{h}} + \frac{Infectives\, \tau}{\left(\mu + \frac{\tau\, Infectives}{h}\right)^2 h}\right)^2 - 2\left(\beta S - \frac{1}{\mu + \frac{\tau\, Infectives}{h}}\right.\right.$$
$$\left.\left. + \frac{Infectives\, \tau}{\left(\mu + \frac{\tau\, Infectives}{h}\right)^2 h}\right)(-\beta\, Infectives - \delta) + (-\beta\, Infectives - \delta)^2 + 4\beta\, Infectives\,(-\beta S - \delta)\right)^{\frac{1}{2}}$$

Example: Simple SITS Model



Associated System of State Equations

$$\dot{S} = -c\left(\frac{I}{S+I+R}\right)\beta S + \frac{R}{\gamma}$$

These represent the same infection flow (flowing out of S, and into I)

$$\dot{I} = c\left(\frac{I}{S+I+R}\right)\beta S - \frac{I}{\mu}$$

These represent the same recovery flow (flowing out of I, and into R)

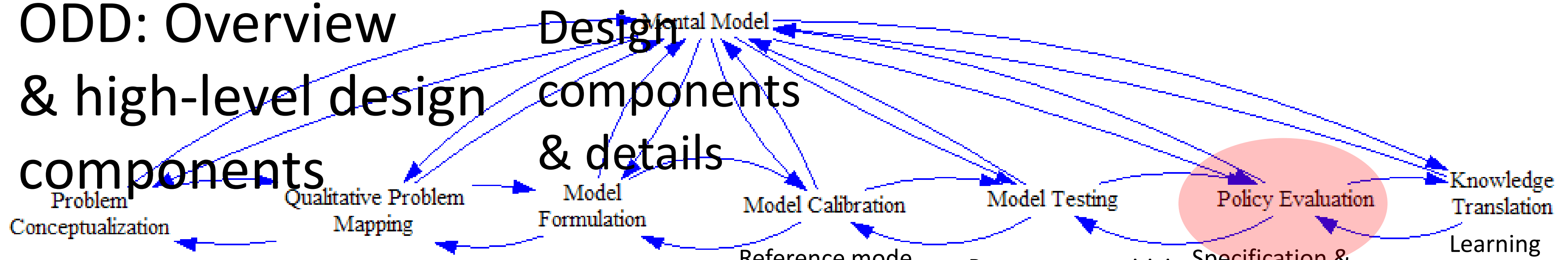
$$\dot{R} = \frac{I}{\mu} - \frac{R}{\gamma}$$

These represent the same loss-of-immunity flow (flowing out of R (hence the minus sign), flowing into S)

ABM Modeling Process Overview

ODD: Overview & high-level design components

ODD: Design components & details



Problem/research question articulation

Patterns for explanation

Model scope/boundary selection (endogeous, exogenous,ignored)

Key entities & their relationships
- Agents (&collectives)
- Environment
- Nesting hierarchy or network diagrams

Output of interest

State charts
Parameter & state variables
Qualitative State charts
Influence & Causal loop diagrams
Multi-agent interaction diagrams
Process flow structure
Key events
Rough model time & spatial extent
Observers to measure outputs

Specification of
- Parameters
- Quantitative causal relations
- Decision/behavior rules
  - Transitions
- Interactions
  - Messaging &handlers
  - Resources
- Relationship dynamics
- Mobility dynamics
- Initial conditions

Reference mode reproduction

Matching of intermediate time series

Matching of observed data points

Constrain to sensible bounds

Structural sensitivity analysis

Parameter sensitivity analysis

Cross-validation
- Formal
- w/Discovered
  - Patterns

Robustness tests

Extreme value tests

Unit checking

Problem domain tests

Specification & investigation of intervention scenarios

Investigation of hypothetical external conditions

Cross-scenario comparisons (e.g. CEA)

Learning environments (e.g. DISimS)

Visualizations

Contact Tracing Simulation

We can make it better!

Run the model and switch to Main view

Network type

- (•) Random
- ( ) Small world
- ( ) Scale free

Network Settings

Connect Per Agent [ ]

Notes: Connects Per Agent is for Random and Small World Networks

Neighbourhood Link Prob [ ]

Notes: Link Prob is for Small World Networks

ScaleFreeM [ ]

Note: ScaleFreeM is for Scale Free Networks

Parameter Settings

Simulation Fraction of RI [ ]

Simulation Fraction of NonRI [ ]

☑ **Enable Database**

Contact Tracing Policy Selection

- (•) No Contact Tracing Program
- ( ) Contact Tracing With Priority

Contact Tracing Priority Settings (Weight)

☑ Age Priority ☑ Ethnicity Priority ☑ RR of Count Priority

Contact Tracing Targets

- (•) Tracing Infectious Active TB Cases ONLY
- ( ) Tracing All Active TB Cases
- ( ) Tracing Infectious Active TB Cases and Primary TB

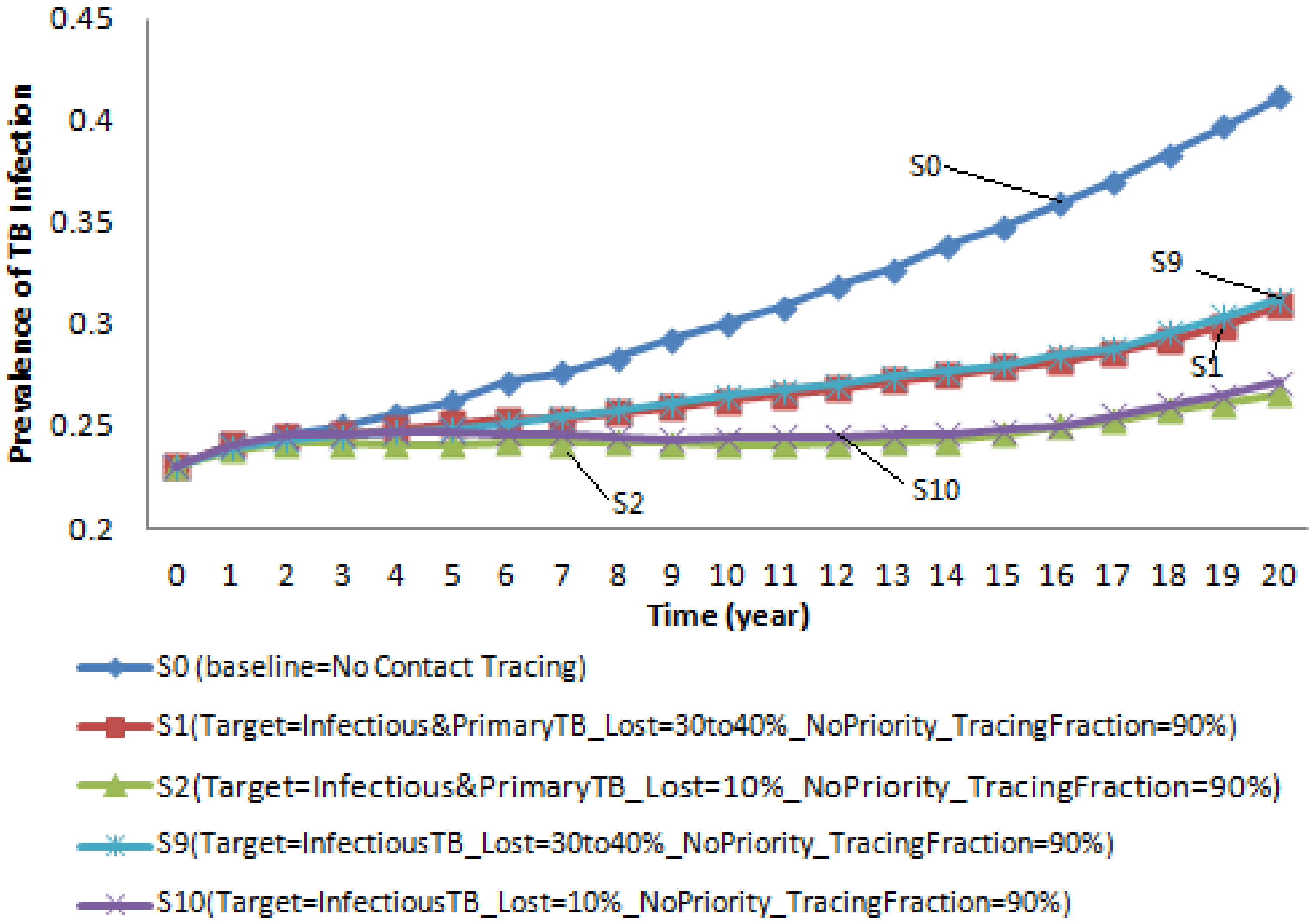
Contact Tracing Percentage on Average

Average Percentage of Contacts to Investigate: [ ]

Scenario Information

Description [ ]

Scenario Results (Means)



Variability in Results

Scenario Id	Cumulative Incident Cases (Active TB)				
	Mean	*Max*	*Min*	*Std. Deviation*	*C.V*
S_0	425.633	614	289	74.659	0.175
S_1	311.767	429	217	49.646	0.159
S_2	279.1	392	211	49.682	0.178
S_3	318.667	403	207	48.093	0.151
S_4	283	364	193	40.403	0.142
S_5	302.233	486	194	64.917	0.215
S_6	363.2	508	239	70.19	0.193
S_7	291	383	190	53.018	0.182
S_8	265.5	400	185	44	0.166
S_9	315	438	184	49.2	0.156
S_{10}	271.6	387	192	41.57	0.153

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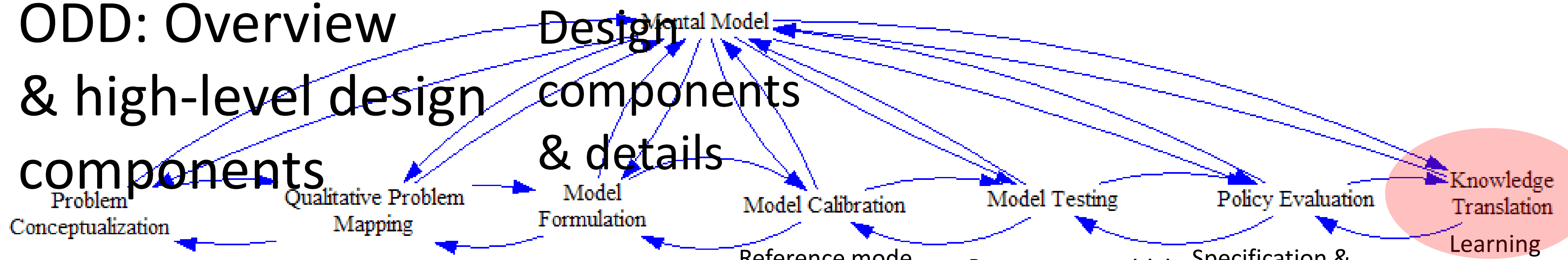

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Key Take-Home Messages from this Lecture

- Models express dynamic hypotheses about processes underlying observed behavior
- Frequently observed behavior is “emergent” – it is qualitatively different than the behavior of any one piece of the system, or a simple combination of behavior of those pieces
- Models help understanding how diverse pieces of system work together
- ABM focus on agent interactions as the fundamental shapers of dynamics
- Models are specific to purpose