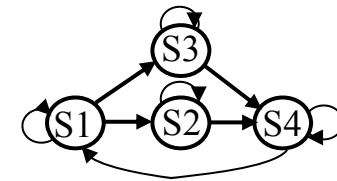
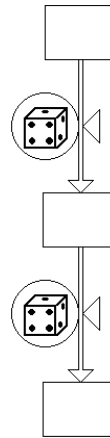
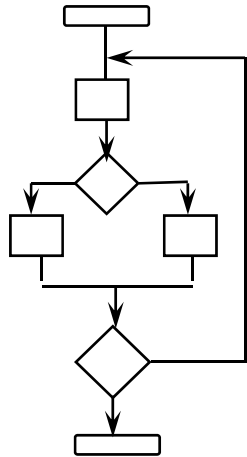


Carpe Systemus*

* System under study

Based on "A Guide to Population Modelling for Simulation"

Mikael Sternad and Leif Gustafsson, Jan. 2019



Internal structure
External structure

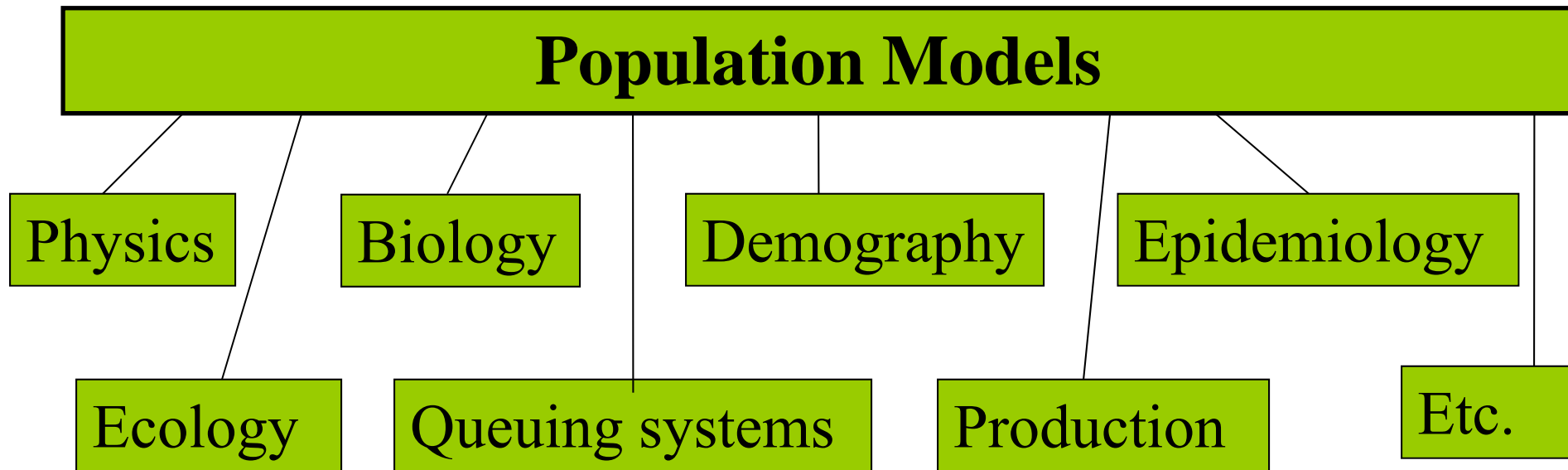
Agent Based Model
(ABM)

Entity Based Model
(EBM)

Compartment Based Model
(CBM)

Situation Based Model
(SBM)

Population models are models based on *discrete entities* such as atoms, molecules, genes, cells, humans, animals, plants etc.



We will here focus on creating (nonlinear) dynamic models that

- are useful for *simulation*,
- where some quantities/state variables are *discrete*, and
- where we often need to use *stochastic* descriptions.

Alternative representations:

Agent-based model (ABM) (Object oriented)
Micro description of each individual (entity).
Individuals may differ in *behaviours* and *attributes*.

Entity-based model (EBM)

Micro description of each individual (entity).
Common behavioural logic – but individuals may differ in *attributes*.

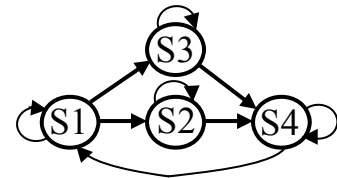
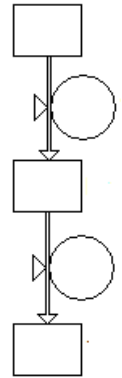
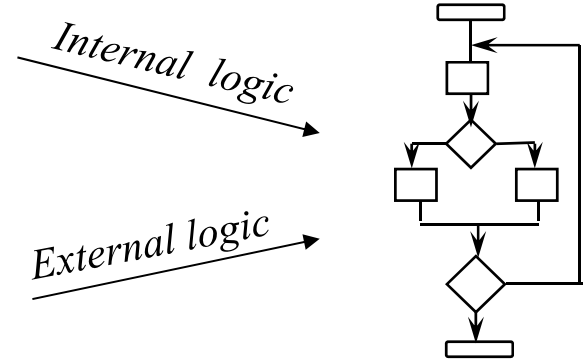
Compartment-based model (CBM)

Macro description of sub-populations.
Similar individuals are *aggregated* into compartments (state variables).

Traditionally *deterministic* models with *continuous* state variables

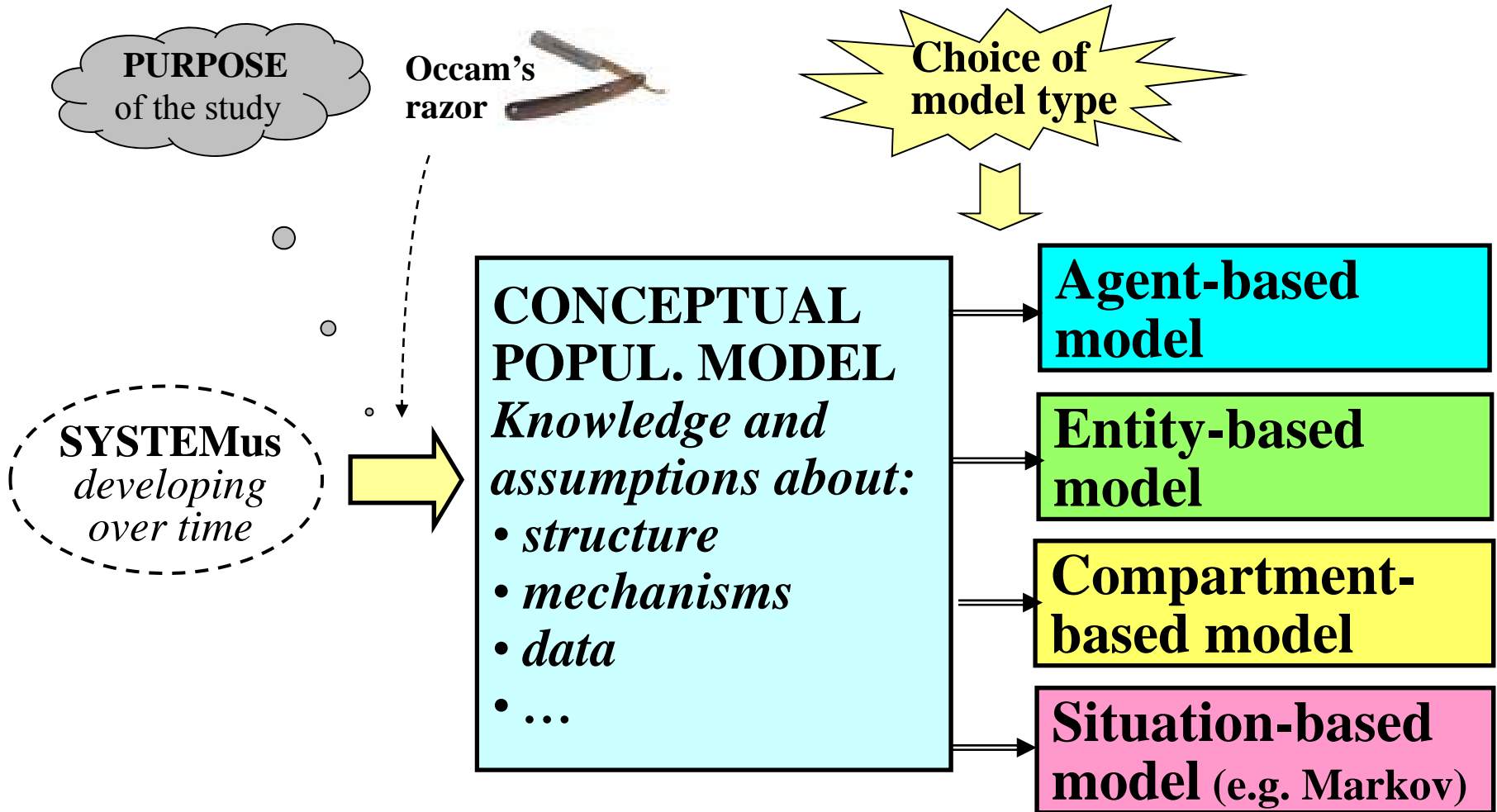
Situation-based model (SBM) (e.g. Markov)

Macro description of all possible *situations* of the conceptual model.
Each and every situation ('state') and *transition* between situations must be described.



System, Conceptual Model and Realisations

TASK: To reproduce a Conceptual model for execution



“All models are wrong, but some are useful.” – for a specific purpose
(George Box)

I. EXAMPE: CONCEPTUAL SIR MODEL

- A population of n individuals is affected by an **infectious disease**, with three consecutive stages:

$$\mathbf{S} \rightarrow \mathbf{I} \rightarrow \mathbf{R}.$$

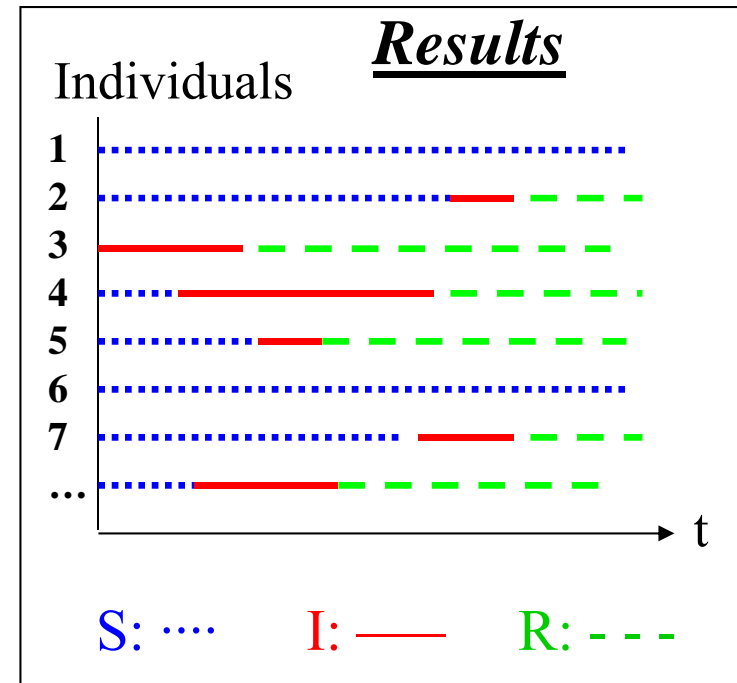
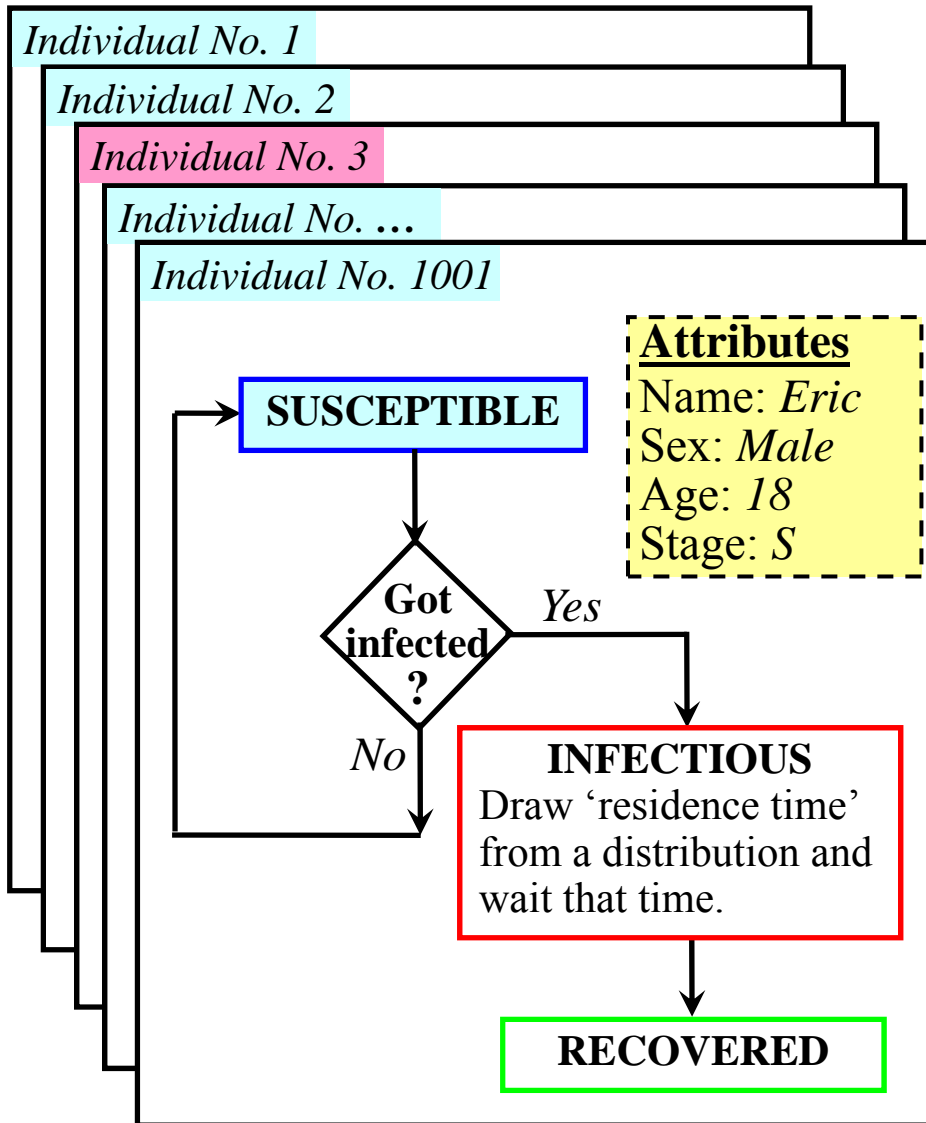
[**S** = Susceptible, **I** = Infectious & **R** = Recovered (and immune)]

- The probability of each Susceptible individual being infected by some Infectious individual is approximated by $p \cdot I$ per time unit (for small p).
 - The expected time in the Infectious stage is T time units.
-
- Usually we will set: $S(0)=1000$, $I(0)=1$, $R(0)=0$, $p=0.0003$, $T=4$.

Agent-based model – SIR example

Each individual is separately modelled (*micro model*) and has:

- 1) **Attributes** (e.g. Name, Sex, Age, Stage of disease, etc.)
- 2) **Behavioural logic** (e.g. Meets other individuals, Gets infected, Recovers, ...)



Epidemic on average ≈ 54.6 persons

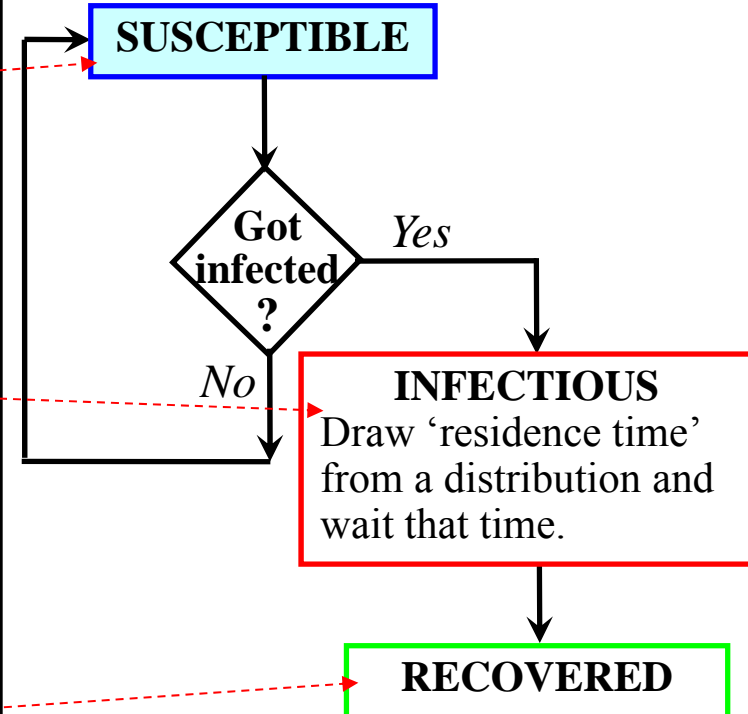
Entity-based model – SIR example

Each individual has Attributes

(e.g. Name, Sex, Age, Stage of disease, etc.)

- But the **Behavioural logic** is common
(e.g. Individuals meet, Infection is transferred, Individuals recover, ...)

All individual have a common logic
(\approx Railway) – but individual attributes.



Attributes

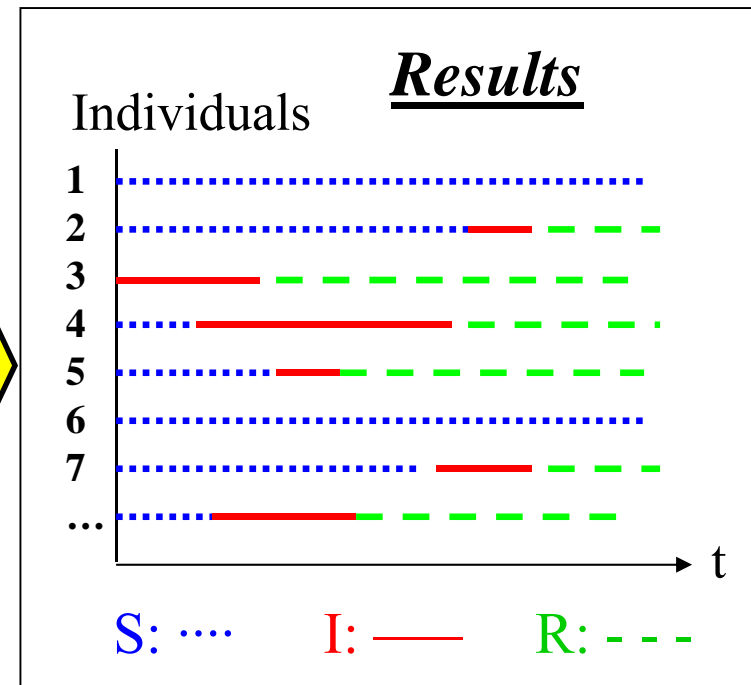
Name: Eric
Sex: Male
Age: 18
Stage: S

Attributes

Name: Ivar
Sex: Male
Age: 42
Stage: I

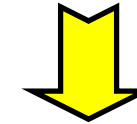
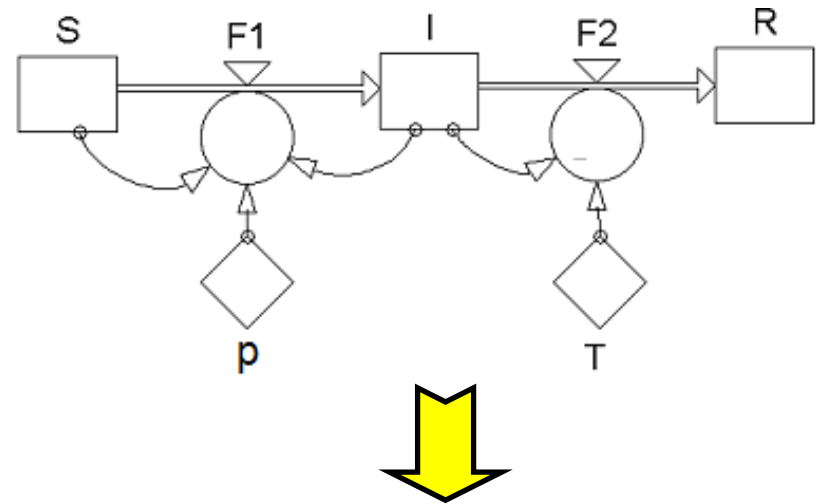
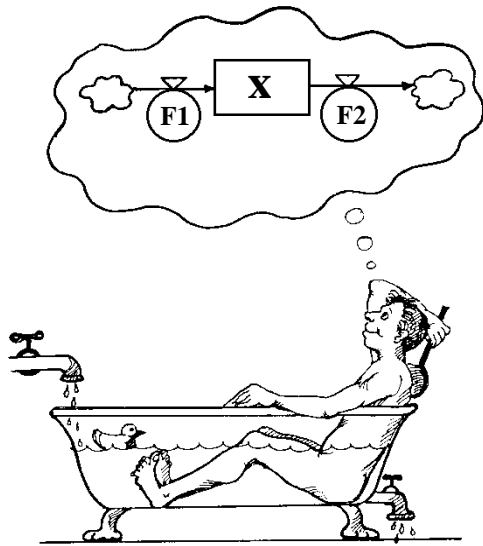
Attributes

Name: Sara
Sex: Female
Age: 23
Stage: R



Epidemic on average ≈ 54.6 persons

Compartment-based model – SIR example

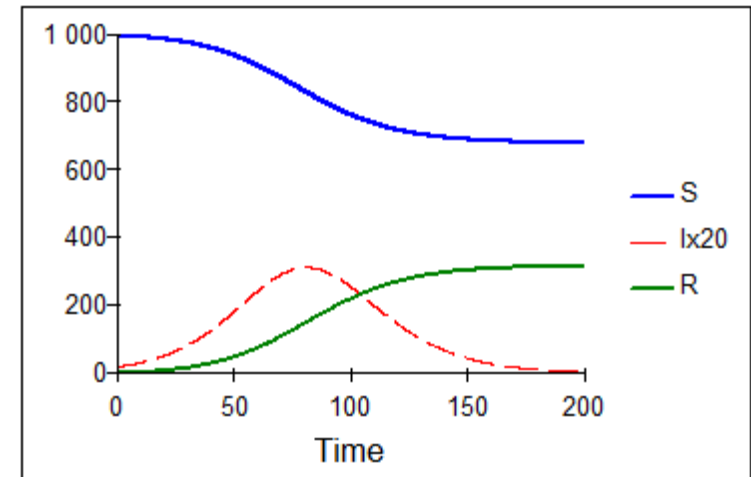


Compartments (state variables):

- **SUSCEPTIBLE (S)**
- **INFECTIOUS (I)**
- **RECOVERED (R)**

“*Macro model*”: Individuals are *not* modelled, only the numbers in each compartment.

Here: $S(t)$, $I(t)$ and $R(t)$ are approximated as **real-valued**, in a **deterministic** model.

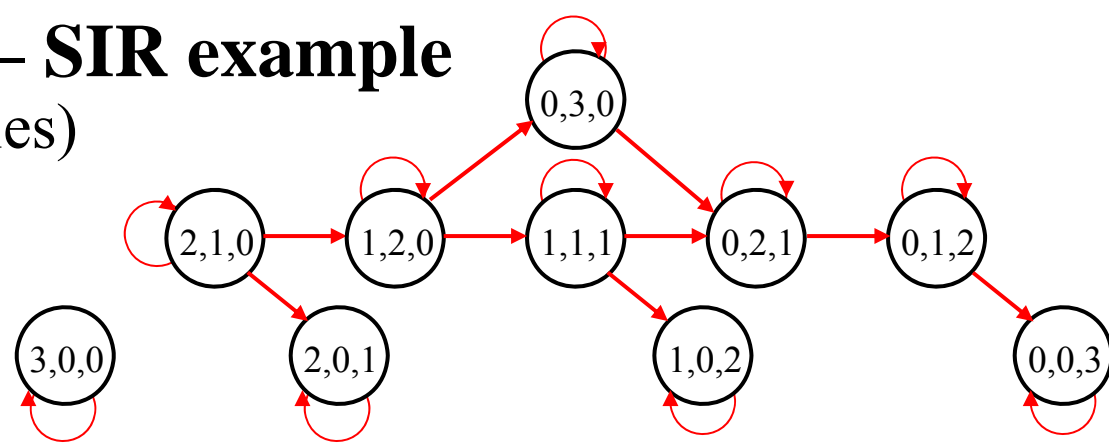


Epidemic ≈ 318.5 persons

Situation-based model – SIR example

(with 3 stages & only 3 entities)

Transition graph:



The transition graph can be represented by a **Transition matrix P**:

	(300)	(210)	(201)	(120)	(111)	(102)	(030)	(021)	(012)	(003)	To situation
(300)	1	0	0	0	0	0	0	0	0	0	(1-Σ means that the row must sum up to unity.)
(210)	0	1-Σ	$h \cdot 1/T$	$h \cdot p \cdot 2 \cdot 1$	0	0	0	0	0	0	
(201)	0	0	1	0	0	0	0	0	0	0	
(120)	0	0	0	1-Σ	$h \cdot 2/T$	0	$h \cdot p \cdot 1 \cdot 2$	0	0	0	
(111)	0	0	0	0	1-Σ	$h \cdot 1/T$	0	$h \cdot p \cdot 1 \cdot 1$	0	0	
(102)	0	0	0	0	0	1	0	0	0	0	
(030)	0	0	0	0	0	0	1-Σ	$h \cdot 3/T$	0	0	
(021)	0	0	0	0	0	0	0	1-Σ	$h \cdot 2/T$	0	
(012)	0	0	0	0	0	0	0	0	1-Σ	$h \cdot 1/T$	
(003)	0	0	0	0	0	0	0	0	0	1	

From situation

State transition relation: $\mathbf{x}(t+h) = \mathbf{x}(t)\mathbf{P}$ can be used for two purposes:

- 1) Propagate the whole pdf (real-valued $\mathbf{x}(t+h)$).
- 2) Simulation: Generate a unique next state (e.g. $\mathbf{x}(t+h) = (0, \dots, 0, 1, 0, \dots, 0)$).
(Epidemic size then depends on step length h)

Conclusions so far...

Micro, Macro and Situation-based models realised from *the same* Conceptual model may produce *different* results!

- Why?
- Can this be fixed? Then how?

II. A NEW VIEW OF MODELLING

ABM, EBM, CBM & SBM realisations of a Conceptual model *can* produce mutually consistent results!

But this requires *understanding* and *following some rules*

Aspects to be discussed briefly:

A. Modelling the distribution of residence times in a stage

B. Time handling

C. Stochasticity and model uncertainty

D. Discrete or continuous matter?

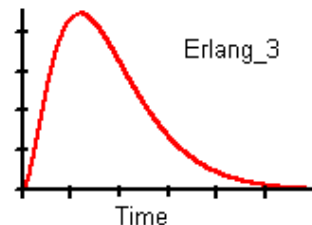
(We need a stochastic CBM where compartments contain integers)

E. Combined simulation (mix of both discrete *and* continuous)

First we need to understand how ABM, EBM, CBM & SBM are related.

Consider a SIR model with:

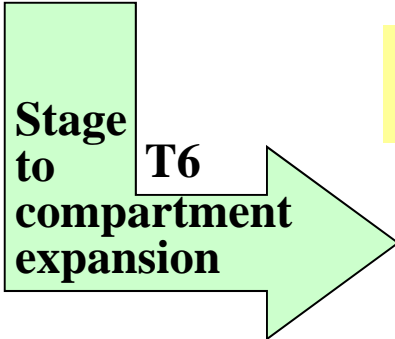
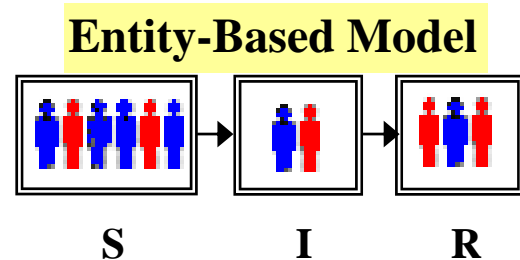
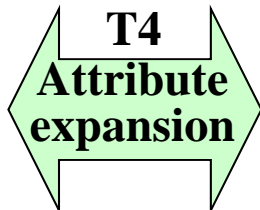
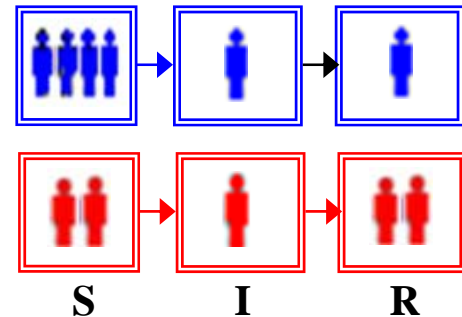
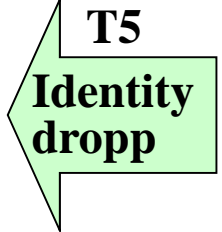
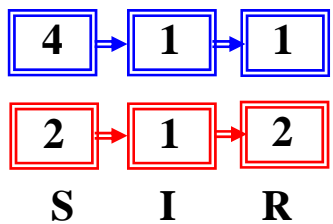
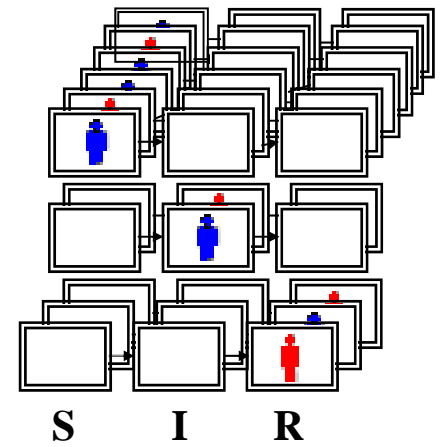
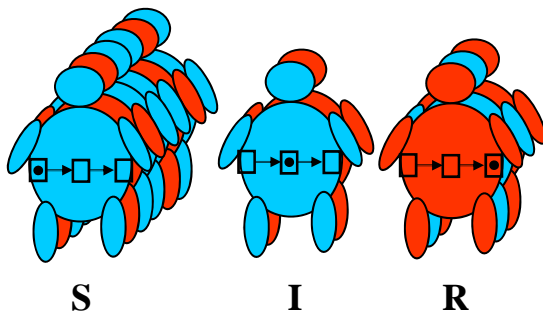
- $n = 6$ males + 5 females. Males and females are here distinguished.
- Residence time in I-stage is a 3-Erlang distribution with average T .



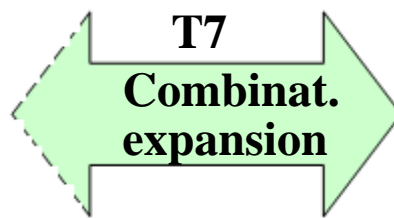
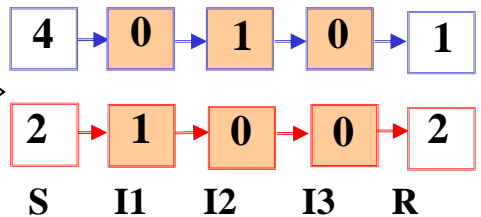
Transformations between model types – SIR model

Agent-Based Model

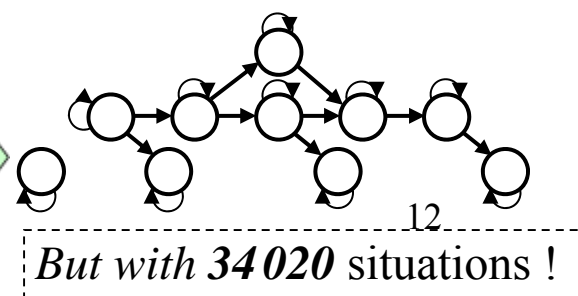
Conceptual SIR model



Stochastic Compartment-Based Model

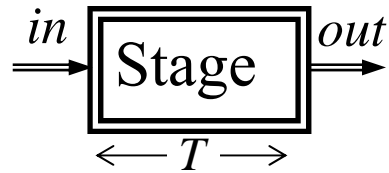


Situation-Based Model

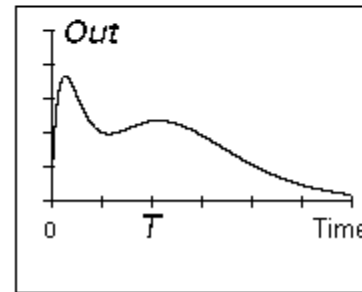
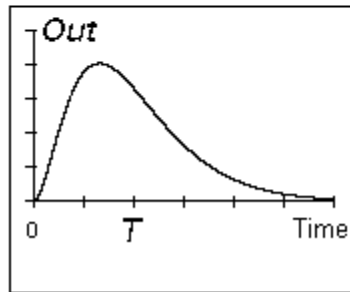
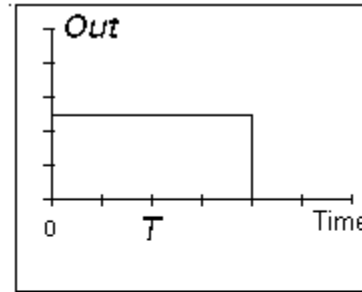
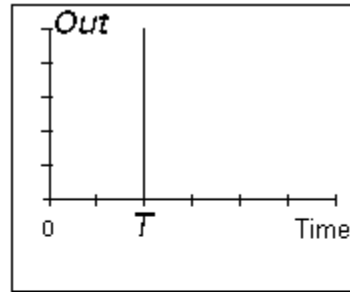
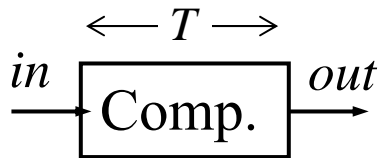


STAGE vs. COMPARTMENT

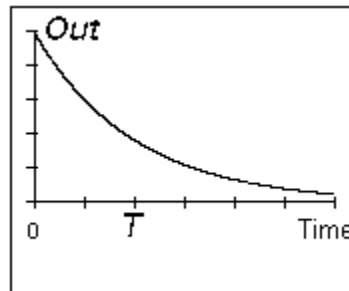
The duration (*Residence time*) in a stage is often not specified deterministically



Same average residence time T .



*A stage has a residence time **distribution** that must be reproduced in the model.*



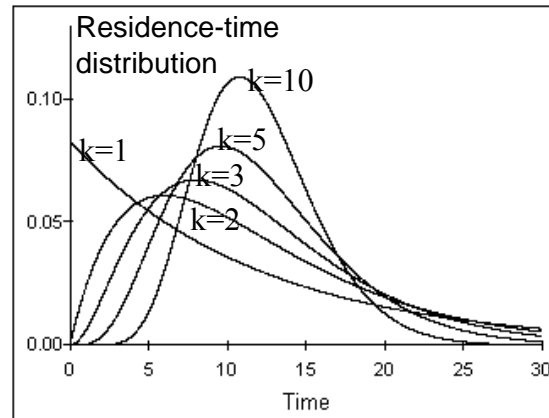
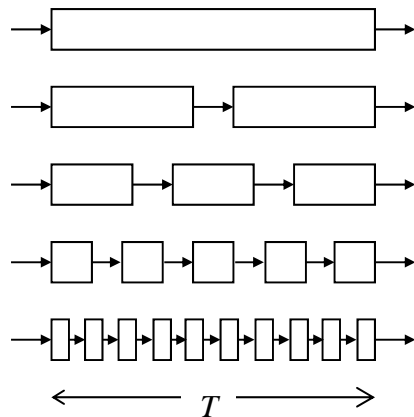
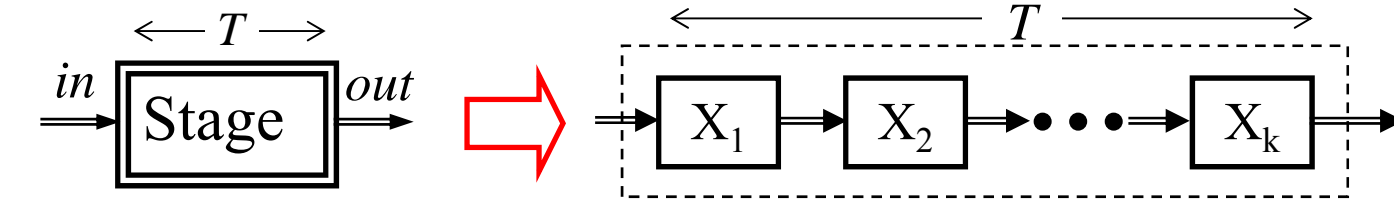
But a single compartment (state variable) always produces an exponential residence-time distribution.

Confusion of Stage and Compartment often gives disastrous consequences!

In CBM, a stage mostly must be represented by a structure of several compartments

- ❑ Residence time distribution equals the normalized (deterministic) impulse response
- ❑ Can be sufficiently approximated by a linear dynamic system structure of compartments in **series** and/or in **parallel**.

Example: A stage (average Residence time = T) is often represented by k serial compartments (each with the time constant T/k).



The k -Erlang(T/k) distribution of the residence time for $k=1, 2, 3, 5$ and 10 compartments.

TIME HANDLING

❑ Event scheduling (to next event)

Only *discrete events* are modelled (by describing what then happens).

- Exactly one event per time step.

❑ Time slicing (Δt)

The model is updated by small *time-steps*.

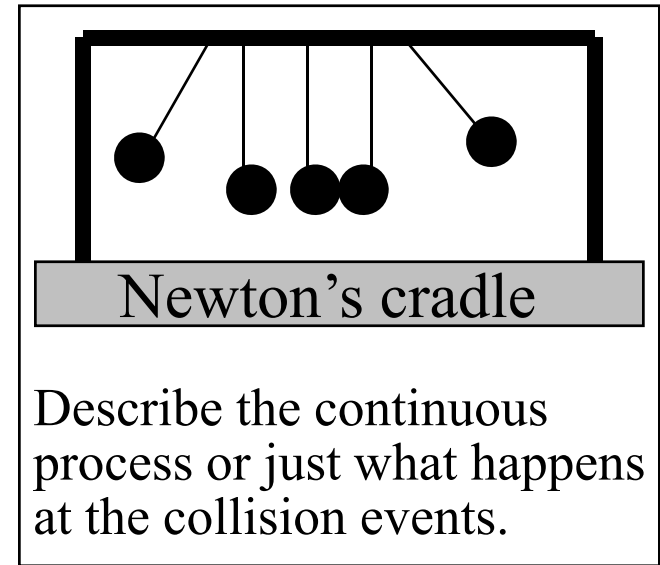
- Many events may occur per time step.

❑ Micro time slicing (h)

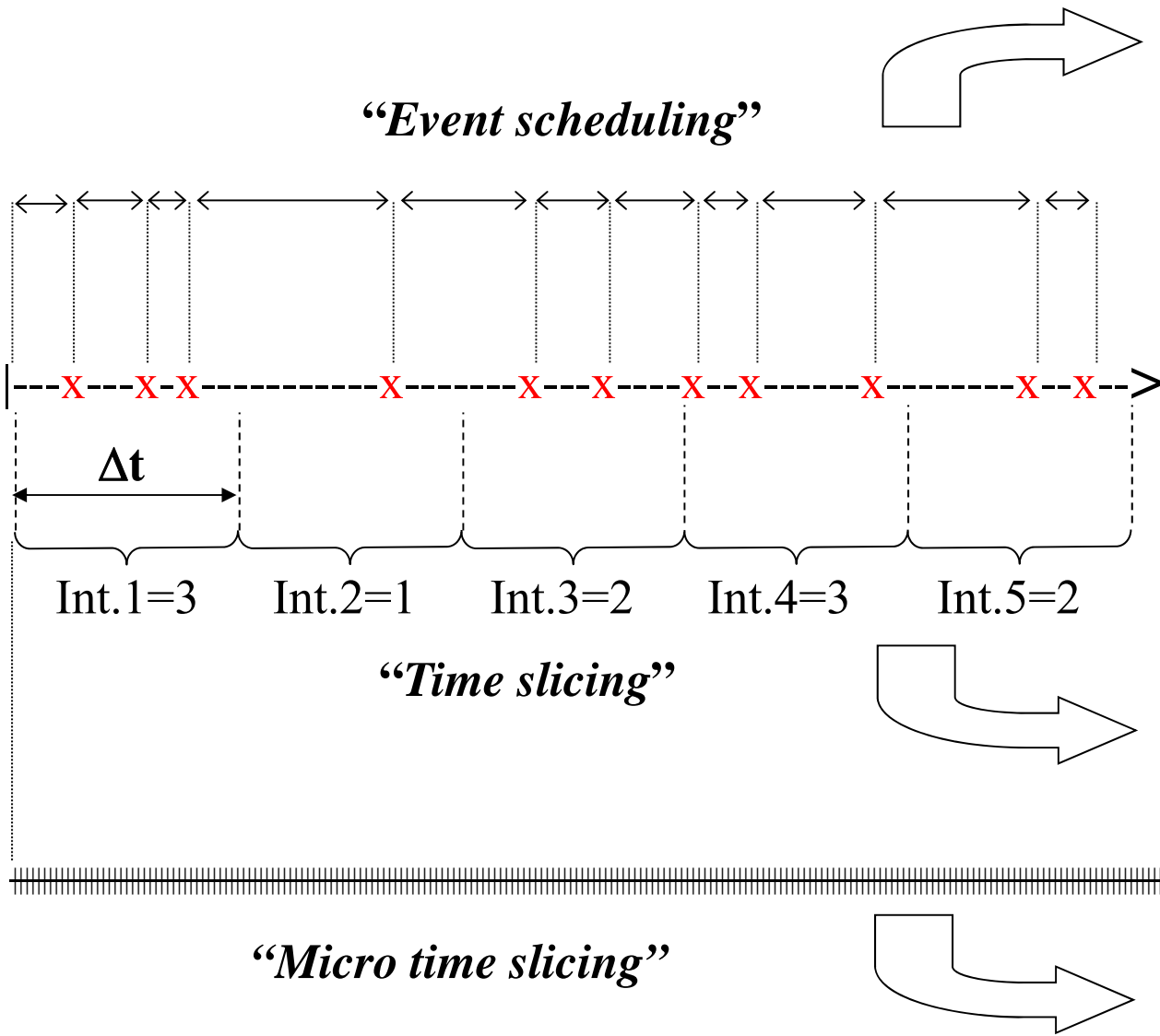
The model is updated with extremely small time-steps.

- Usually zero and occasionally one event occurs per time step.

(Also used mathematically for diff. equations, $\lim h \rightarrow 0$).



Time-handling principles



Exponential distribution
of time between events
 $\text{Exp}[-\lambda]$.
(ABM & EBM)

Independent events (x)
over time, with constant
probability λ per time unit.

Poisson distribution
($\Delta t = \text{Length of interval}$)
 $\text{Po}[\Delta t \cdot \lambda]$.
(CBM)

Bernoulli distribution
($h = \text{Length of interval}$)
 $\text{Ber}[h \cdot \lambda]$
(where $h \cdot \lambda \ll 1$).
(SBM)

Representation and time handling principles can be freely combined

	Entity-based	Compartment-based	Situation-based
Event scheduling	DES ¹ (1959)	SSA ² (1976)	Markov jump model
Time slicing (Δt)	(sometimes very useful)	PoS ³ (2000)	(Markov model)
Micro time slicing (0 or 1 ev./h)	(possible but stupid)	(possible but stupid)	Markov model (1906)
<i>lim analysis</i> $h \rightarrow 0$		ODEs	Stat. Analysis

1) DES: Discrete System Simulation

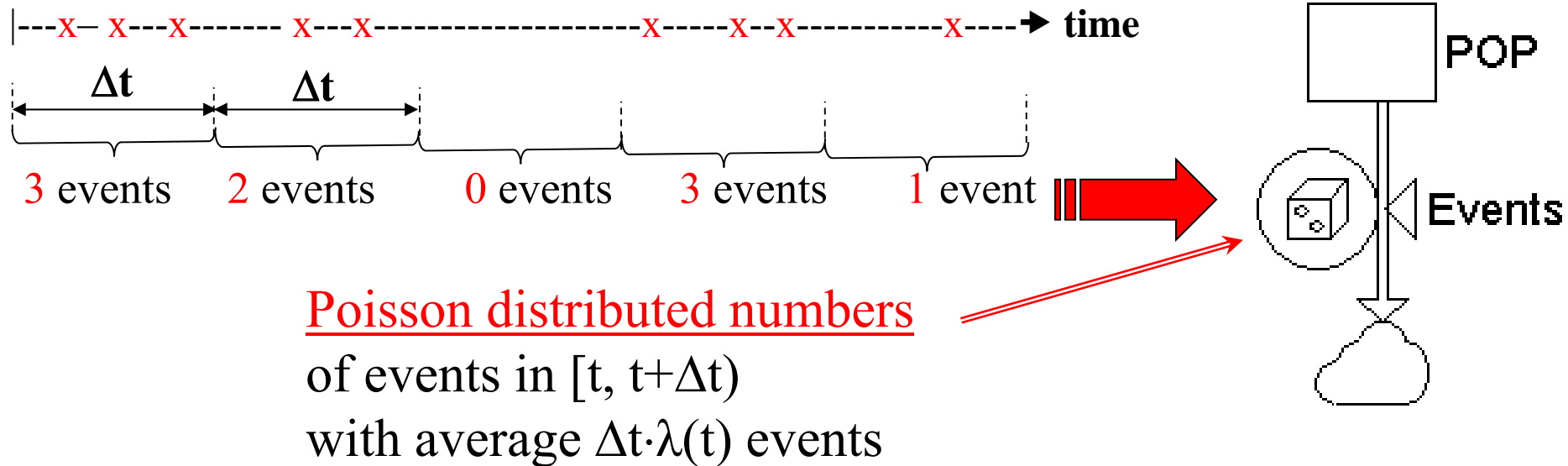
2) SSA: Stochastic Simulation Algorithm

3) PoS: Poisson Simulation (Tau-leap simulation)

Poisson Simulation (PoS)

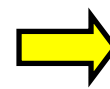
(Stochastic compartment-based modelling with time-slicing)

Random distribution of events over time (slowly time-varying $\lambda(t)$)



1. Set $\text{Pop}(t=0) = \text{integer}$

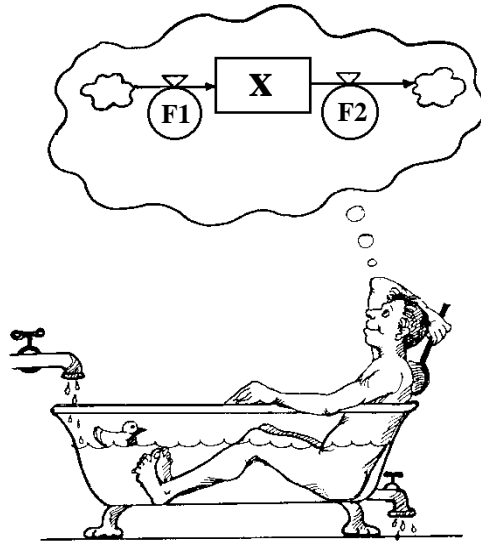
2. The number of events from the Po-distribution is always integer



POP(t) will stay integer for all time.

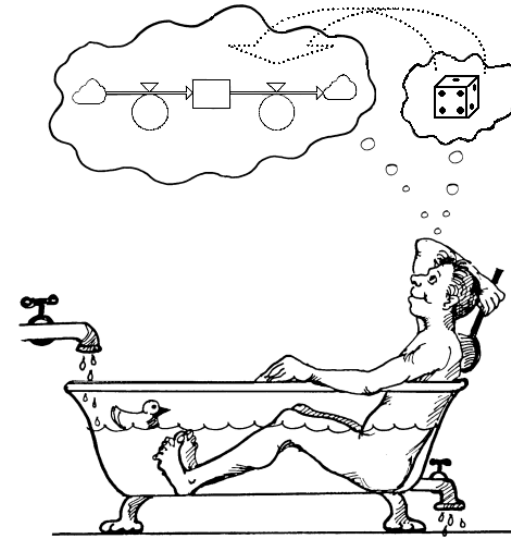
Deterministic and stochastic CBMs

Deterministic compartment-based model



$$\begin{cases} X(t+\Delta t) = X(t) + \Delta t \cdot F1 - \Delta t \cdot F2 \\ \Delta t \cdot F1 = \Delta t \cdot \text{input}(t) \\ \Delta t \cdot F2 = \Delta t \cdot \text{output}(t) \end{cases}$$

Stochastic compartment-based model



$$\begin{cases} X(t+\Delta t) = X(t) + \Delta t \cdot F1 - \Delta t \cdot F2 \\ \Delta t \cdot F1 = \mathbf{Po}[\Delta t \cdot \text{input}(t)] \\ \Delta t \cdot F2 = \mathbf{Po}[\Delta t \cdot \text{output}(t)] \end{cases}$$

Combined simulation in CBM

A combined Volterra model where:

X = prey = grass (continuous state variable)

Y = no. of predators = sheep (discrete).

$$\Delta X = \Delta t \cdot (Rb - Rk - Rd)$$

$$\Delta t \cdot Rb = a \cdot X \quad (\text{birth})$$

$$\Delta t \cdot Rk = k \cdot X^2 \quad (\text{competition})$$

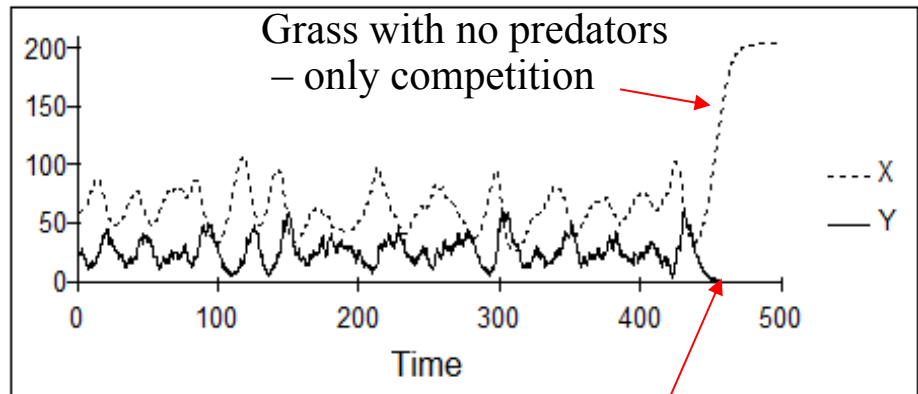
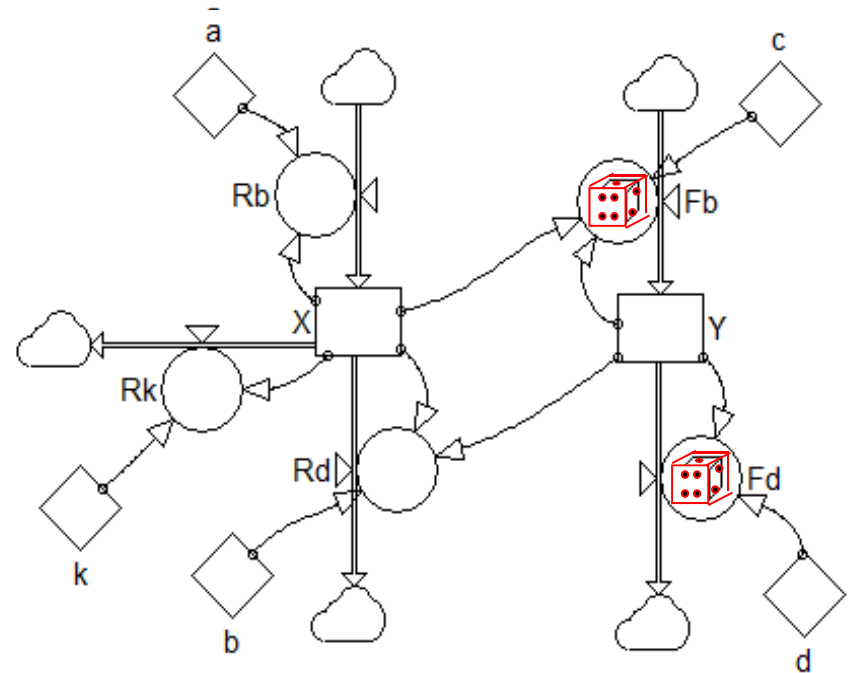
$$\Delta t \cdot Rd = b \cdot X \cdot Y \quad (\text{death})$$

$$\Delta Y = \Delta t \cdot (Fb - Fd)$$

$$\Delta t \cdot Fb = \mathbf{Po}[\Delta t \cdot c \cdot X \cdot Y] \quad (\text{birth})$$

$$\Delta t \cdot Fd = \mathbf{Po}[\Delta t \cdot d \cdot Y] \quad (\text{death})$$

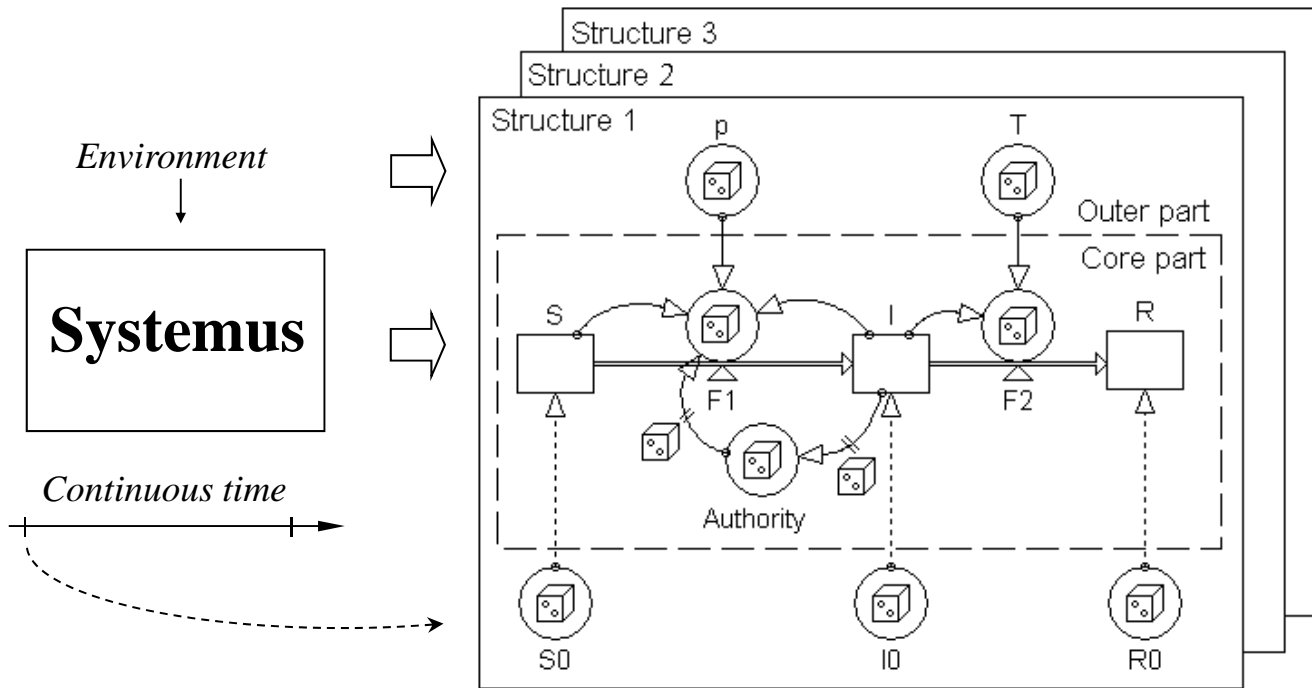
Note the elegance of combining continuous and discrete processes in the same model!



Sheep extinction

Capturing modelling uncertainty

Stochastic models (Also with alternative structures, *structural uncertainty*)



- **Parameter stochasticity** (“environmental”)
- **Transition stochasticity** (“demographic”)
- **Information stochasticity**
- **Initial-value stochasticity**

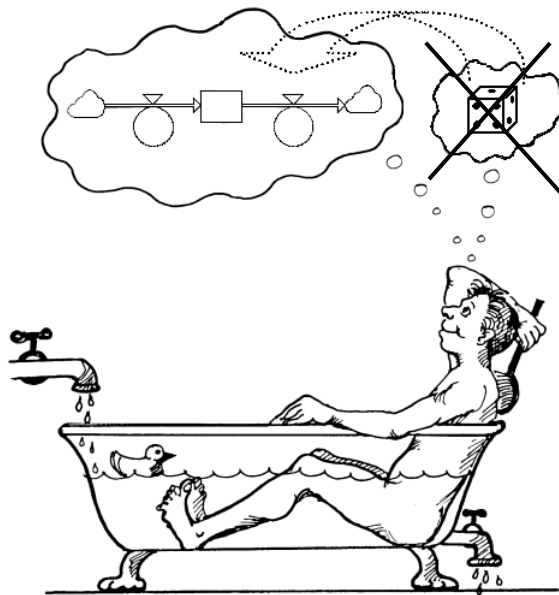
Dice represent where different types of stochasticities can be included in the model

- An epidemic system under study
- Several possible models: Structure 1 is a SIR model based on the stages S , I and R , with Infected stage modelled by a single compartment. (Other Structures use more states.)

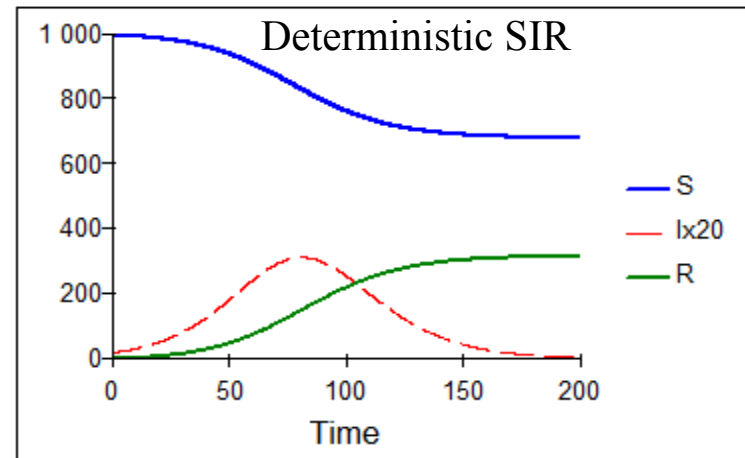
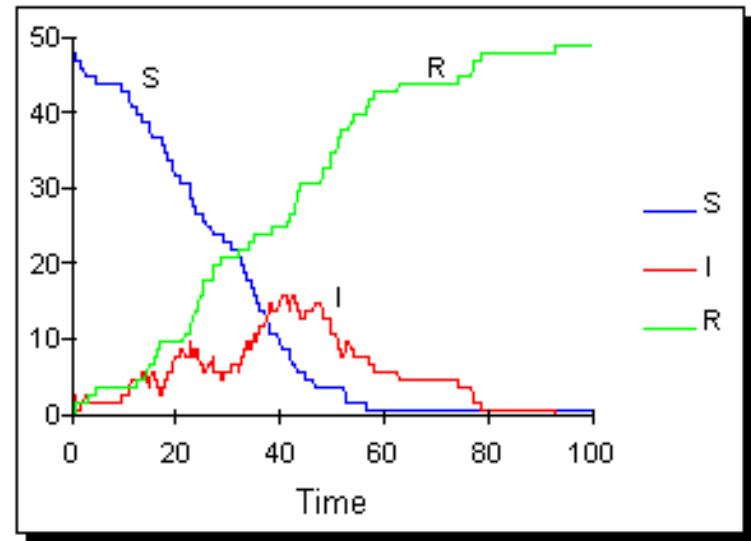
Also added here: An ‘Authority’, which monitors and affects the infection rate. 21

III. CAN WE DROP STOCHASTICS IN A CBM?

Conceptual Model

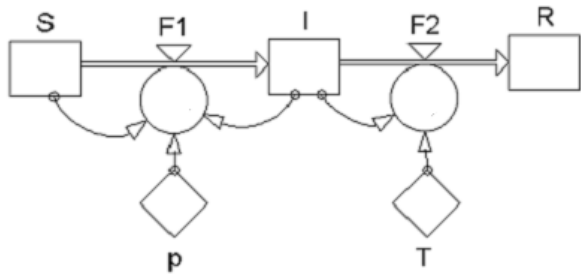


Deterministic CBM

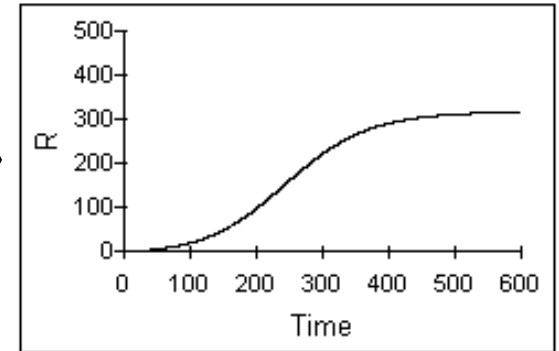


Deterministic vs. Stochastic SIR model

where $S(0)=1000$, $I(0)=1$ & $R(0)=0$ and $p=0.0003$, $T=4$ time units.

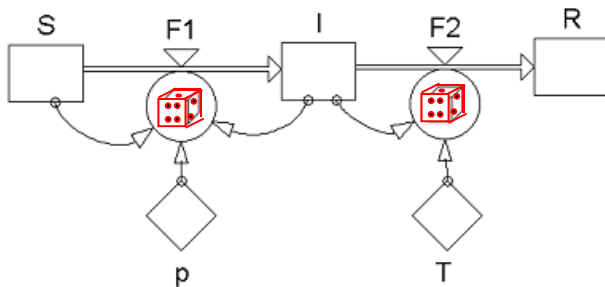


$$\begin{cases} S := S - \Delta t \cdot F_1 \\ I := I + \Delta t \cdot F_1 - \Delta t \cdot F_2 \\ R := R + \Delta t \cdot F_2 \\ F_1 := p \cdot S \cdot I \\ F_2 := I/T \end{cases}$$

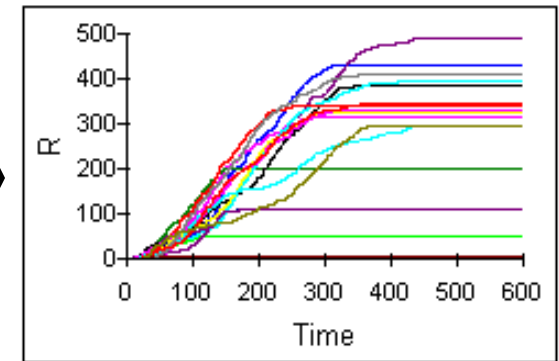


Always an epidemic!

Epidemic size ≈ 318.5 persons



$$\begin{cases} S := S - \Delta t \cdot F_1 \\ I := I + \Delta t \cdot F_1 - \Delta t \cdot F_2 \\ R := R + \Delta t \cdot F_2 \\ F_1 := \text{Po}[\Delta t \cdot p \cdot S \cdot I] / \Delta t \\ F_2 := \text{Po}[\Delta t \cdot I / T] / \Delta t \end{cases}$$

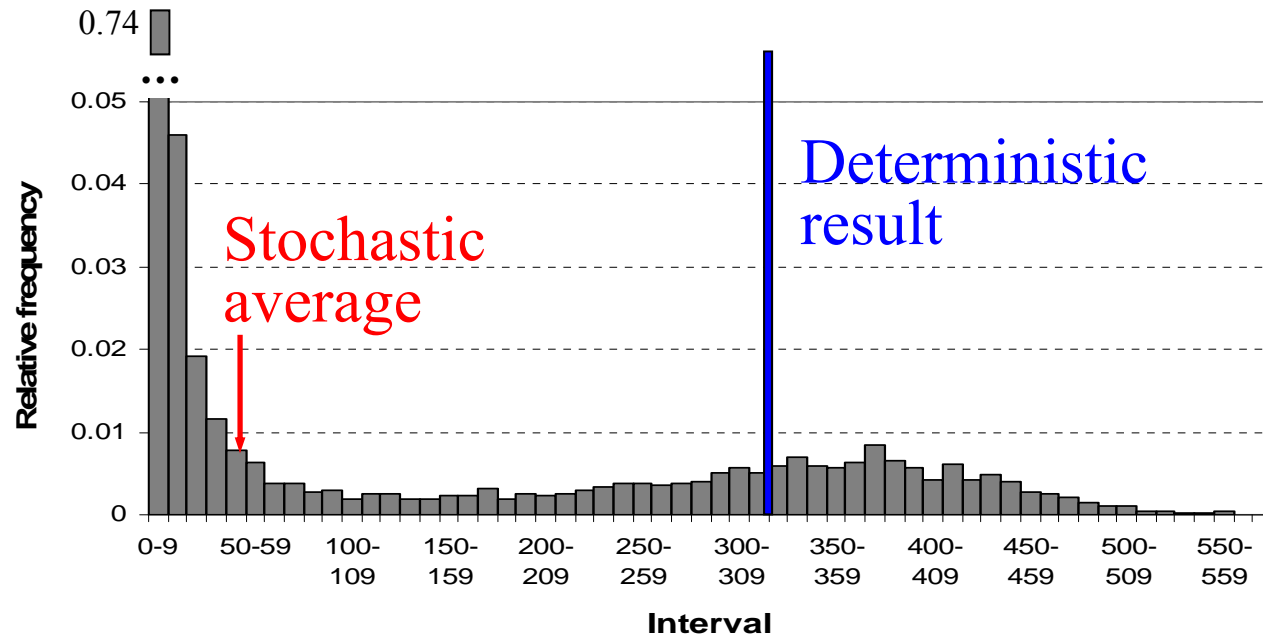


50 replications – mostly no epidemic!

Average epidemic size ≈ 54.6 persons

Deterministic vs. Stochastic SIR model – cont.

Pdf over the number of infected individuals in $10\,000$ replications.



The deterministic population model generates a *biased result* in this case: Its epidemic size differs from the average epidemic size generated by the corresponding stochastic model.

The difference is mainly due to that epidemics will often never get started at all in the stochastic case. This never occurs in the deterministic model!

When will a deterministic population model produce unbiased results?

1. For a *linear* dynamic population system, a deterministic model will produce unbiased results as long as *all compartments remain non-negative* for both the deterministic and the (demographically) stochastic model.

This also requires that the question under study is compatible with *a solution over a fixed time interval*.

2. If *the flows* in a model with demographic stochastics *stay large* and *if the local linearised dynamics is asymptotically stable*, then unbiased results are approached in the limit of large flows.

Testing a deterministic model for bias:

- *Run the stochastic model for, say, 10,000 simulation runs.*
- *Then run the deterministic model once.*
- *Compare whether the outcome is within the confidence interval of the stochastic results.*

IV. CHOICE OF MODEL TYPE

The appropriate choice of model type (ABM, EBM, CBM or SBM) can often be the difference between a smooth and successful project versus hard work and a failure!

There are several aspects to consider:

Micro or macro problem?

Lucid & pedagogic

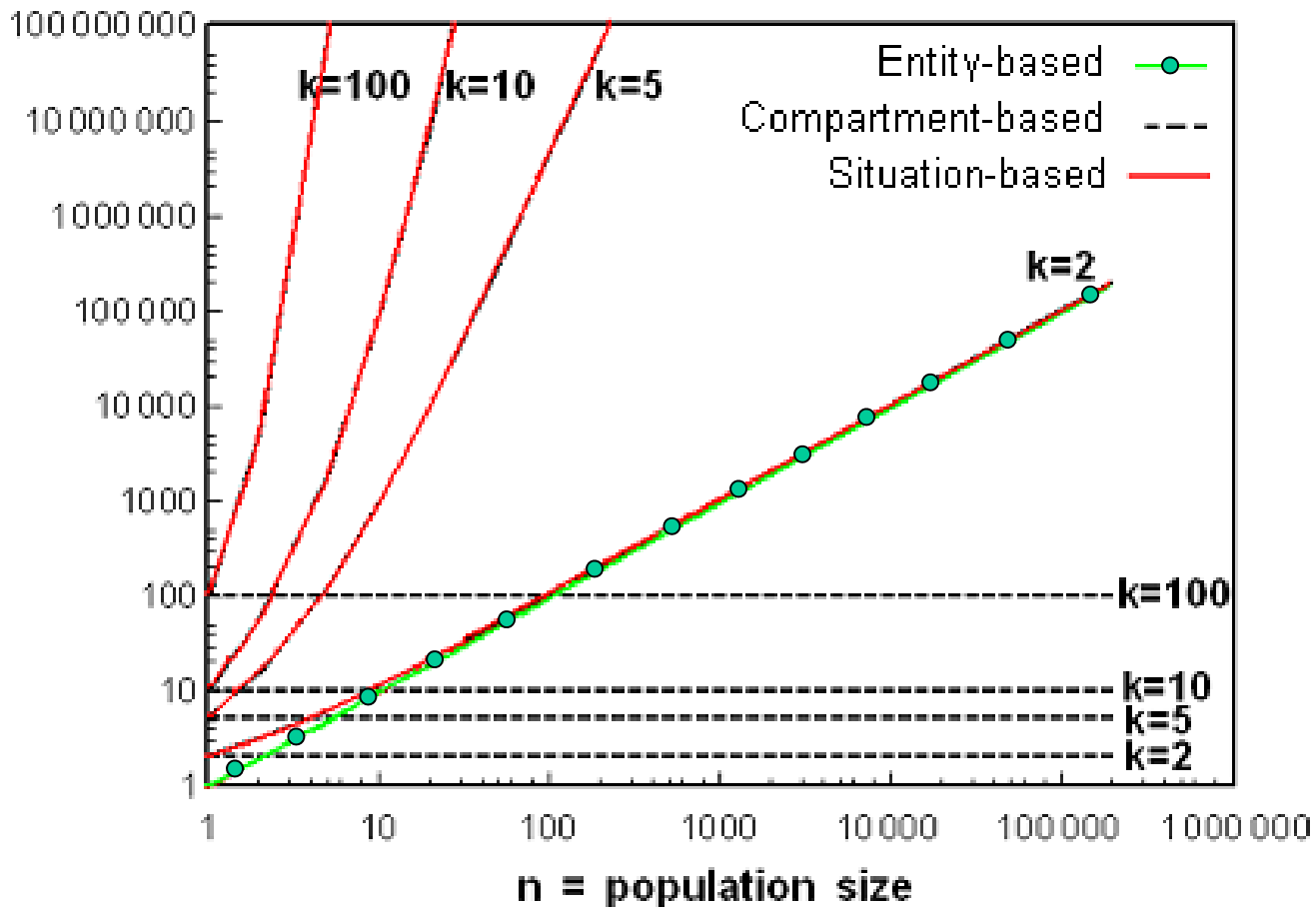
Appropriate size of model?

Easy to build, fit, validate and handle

The access to data (e.g. individual or aggregated) is also important

...

Model size for different representations



The number of elements in a model is a good proxy for its size.

Entity-based: Number of individuals

Comp.-based: Number of compartments

Situation-based: Number of situations

The number of **situations** (for a closed population) is: $\frac{n+k-1}{k-1} = \frac{(n+k-1)!}{[n! \cdot (k-1)!]}$

Which model representation to choose?

- **Stochastic compartment-based models** are usually simplest for most studies of populations when you are *not* primarily interested in the individual, e.g. in epidemiology or ecology.

Deterministic CBM (when not distorting results) can be very nice

- One simulation instead of many
- Often partly analytical (e.g. equilibrium obtained from $d\underline{x}/dt=0$).

- **Agent & Entity-based models** are required:

- 1) For *heterogeneous models* (with many attributes).
- 2) *When you need a micro perspective to follow individuals.*
- (3) Are usually best when a continuous attribute space (e.g. geographical locations) is involved.

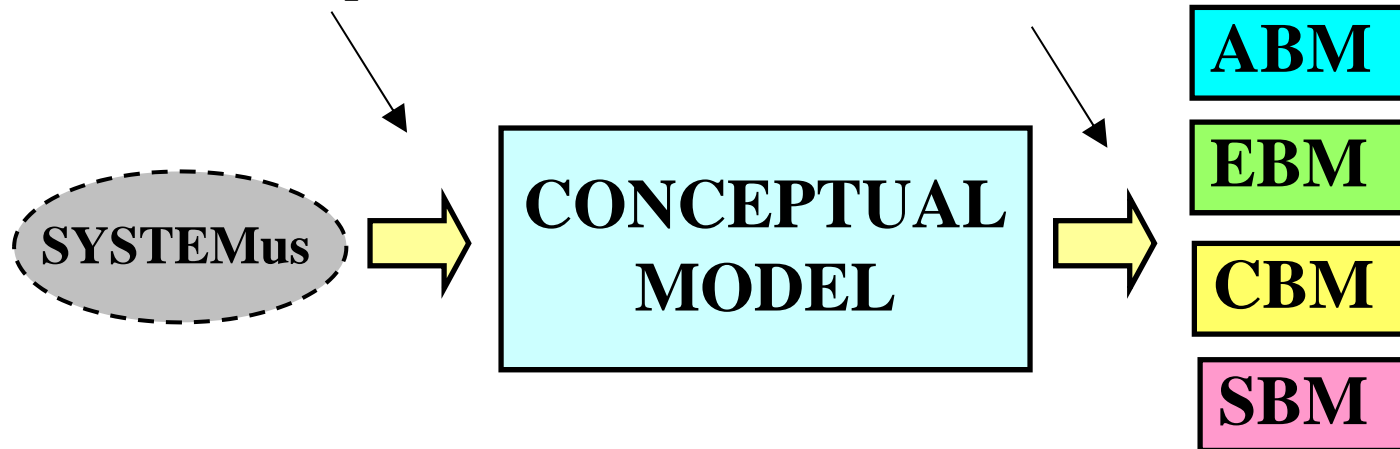
- **Situation-based models** are *never* a good choice for simulation!
(But they have powerful analytical features that can be useful for very small models.)

V. CONCLUSION

*“All models are wrong,
but some are useful”*

Refers to this step

... not to this step!



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END

Extra slides

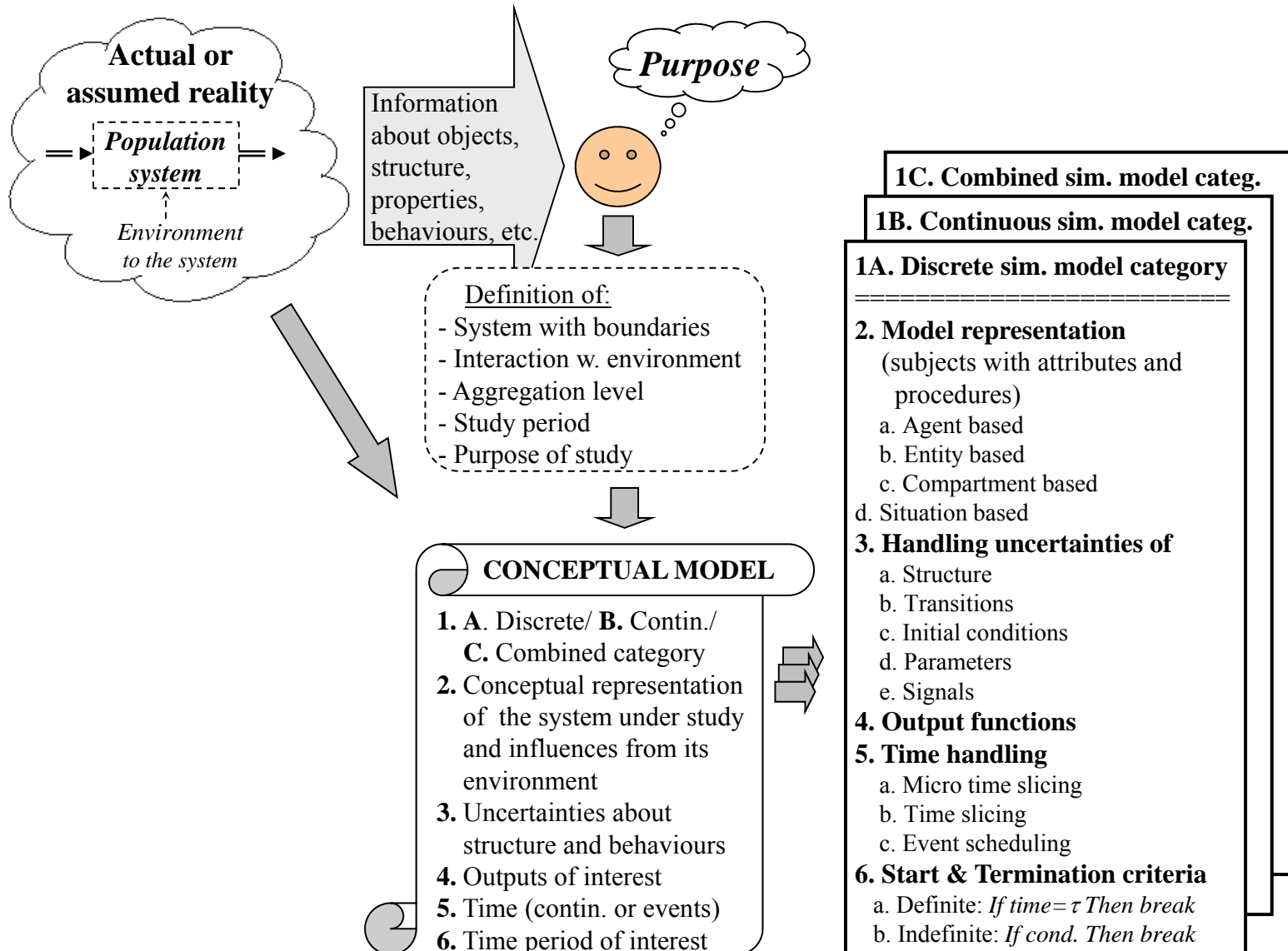
SYSTEMS WORLD

CONCEPTUAL WORLD

“What to do”

SIMULATION MODELS WORLD

“How to do it”



THE OLD VIEW OF MODELLING

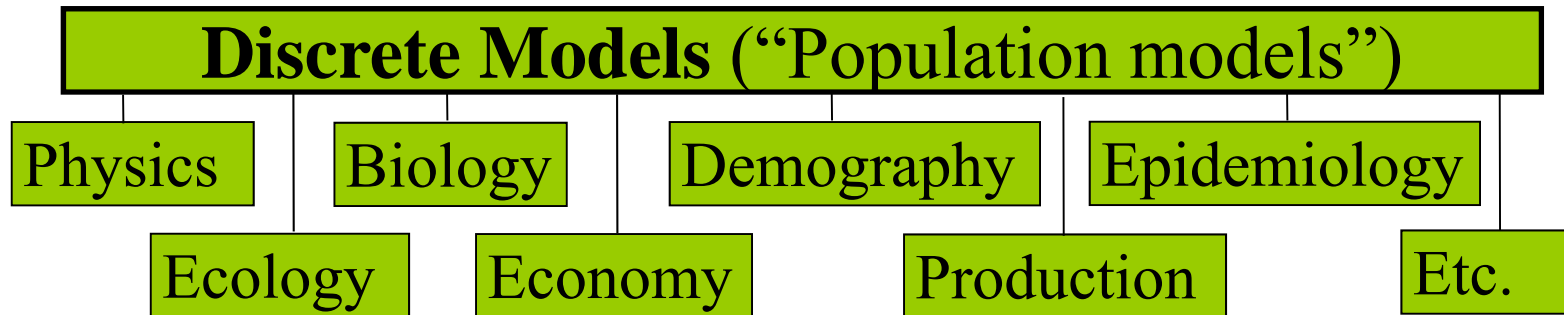
	ABM & EBM	CBM	SBM (Markov)
WORLD VIEW	<i>Micro:</i> Individuals ($n \in \mathbb{N}$)	<i>Macro:</i> Amounts stored in compartments ($x \in \mathbb{R}$)	Extreme decompo- sition into every situation the model can take ($s \in \mathbb{N}$)
COMPO- NENTS	Actors/entities and Resources	Compartments and flows	Situation vector & Transition matrix
DYNAMICS	Programmed behaviour (Flowchart)	System of diff. Equations ($\underline{dx}/dt=f(\underline{x}, t)$)	Matrix multiplication based on the Markov condition
TIME	Discrete events	Continuous (almost)	Fixed time step
RANDOM	Usually of central importance	Usually no randomness	Conditional probab.
RESULTS	Statistics accumulated during a simulation	Time functions $x=f(t)$	How the situations (states) develop
LANGUAGE	General program lang. + Discrete event handler, Actors, Resources, etc.	Program package for integr. of dif. equations + Functions, etc.	Mathematical matrix operations

Unfortunately they often produce *inconsistent* results and conclusions

A) Discrete or continuous modelling

ABM, EBM & SBM are by nature discrete. *Transitions are based on probabilities.*

Discrete models use a *micro view* of atoms, molecules, genes, cells, humans, animals, plants etc.

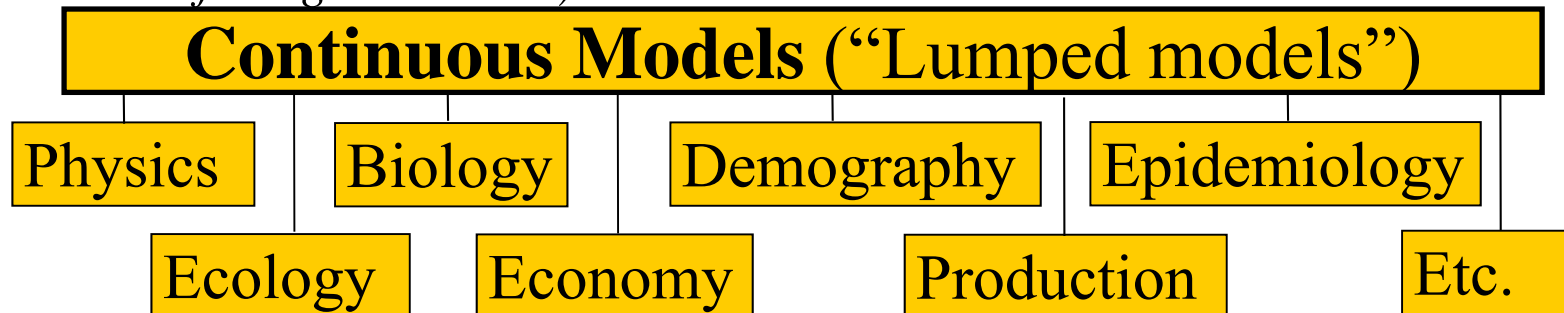


CBM (ODE) is by nature continuous. *Transitions are based on fractions.*

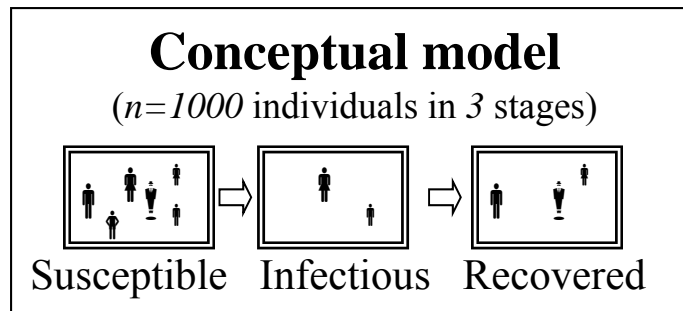
Continuous models use a *macro view* of very large numbers of atoms, molecules, genes, cells, humans, animals, plants etc.

When $n \rightarrow \infty$ then Std. dev. = $1/\sqrt{n} \rightarrow 0$, why stochasticity can be dropped.

(The Law of Large Numbers)



Agent/Entity, Comp. & Situation-based models



Focus on: a) *Individuals* b) *Number in various stages* c) *Situations*

Agent or Entity-based

Agent/ Entity	Attribute (S, I or R)
1	S
2	S
3	I
4	S
5	R
...	...
...	...
999	R
1 000	S

n=1 000 entities

Compartment-based

# Susc.	# Infect.	# Recov.
837	7	156

k=3 compartments

Situation-based

State No.	Comb. (S,I,R)
0	(1000, 0, 0)
1	(999, 1, 0)
2	(999, 0, 1)
3	(998, 2, 0)
4	(998, 1, 1)
5	(998, 0, 2)
6	(997, 3, 0)
...	
...	
13 522	(837, 7, 156)
...	
501 501	(0, 1, 999)
501 501	0, 0, 1000)

Present situation →

501 501 situations

Feasible and unfeasible distribution of residence time

Most processes in real life require a finite time to be performed

- For e.g. biological/medical processes a finite time is needed for digesting, transportation of nutrients, defeating a disease, developing a cancer, growing an embryo, etc.

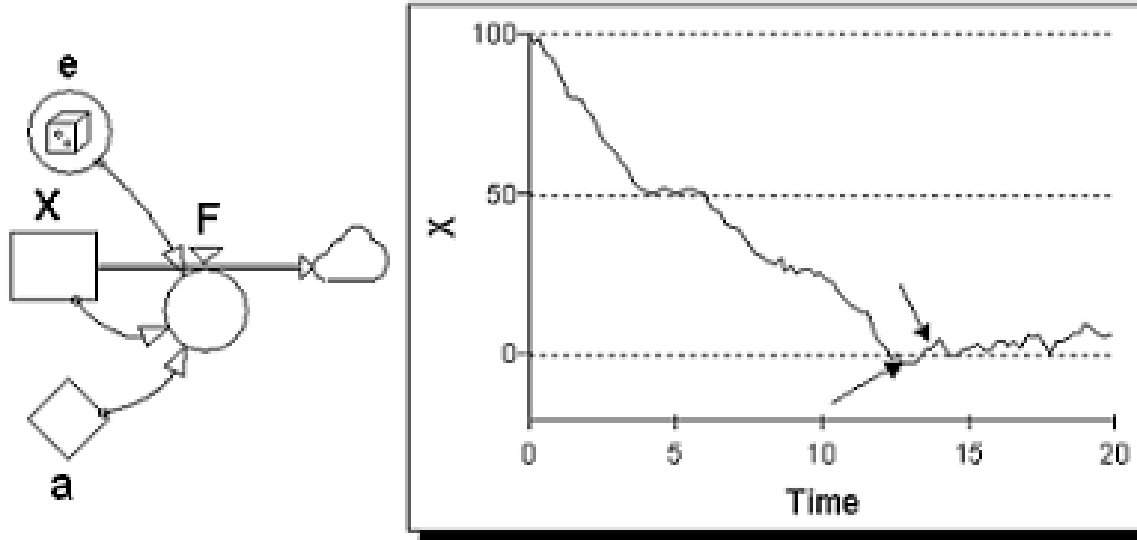
- For such a process a first order process is biologically unfeasible because it means that the probability of performing the process in almost zero time, i.e. finishing it within $(0, \varepsilon)$, is larger than finishing it in any other time interval $(t, t + \varepsilon)$ of length ε .

- Only a few non-biological processes, like radioactive decay, may be accurately modelled with a single compartment (exponentially distributed residence time).

Why not just add noise to a deterministic model?

Ex: *Radioactive decay with $\Delta x(t) = -ax(t)\Delta t + e(t)\Delta t$*
(where $e(t)$ is Normal distributed white noise.)

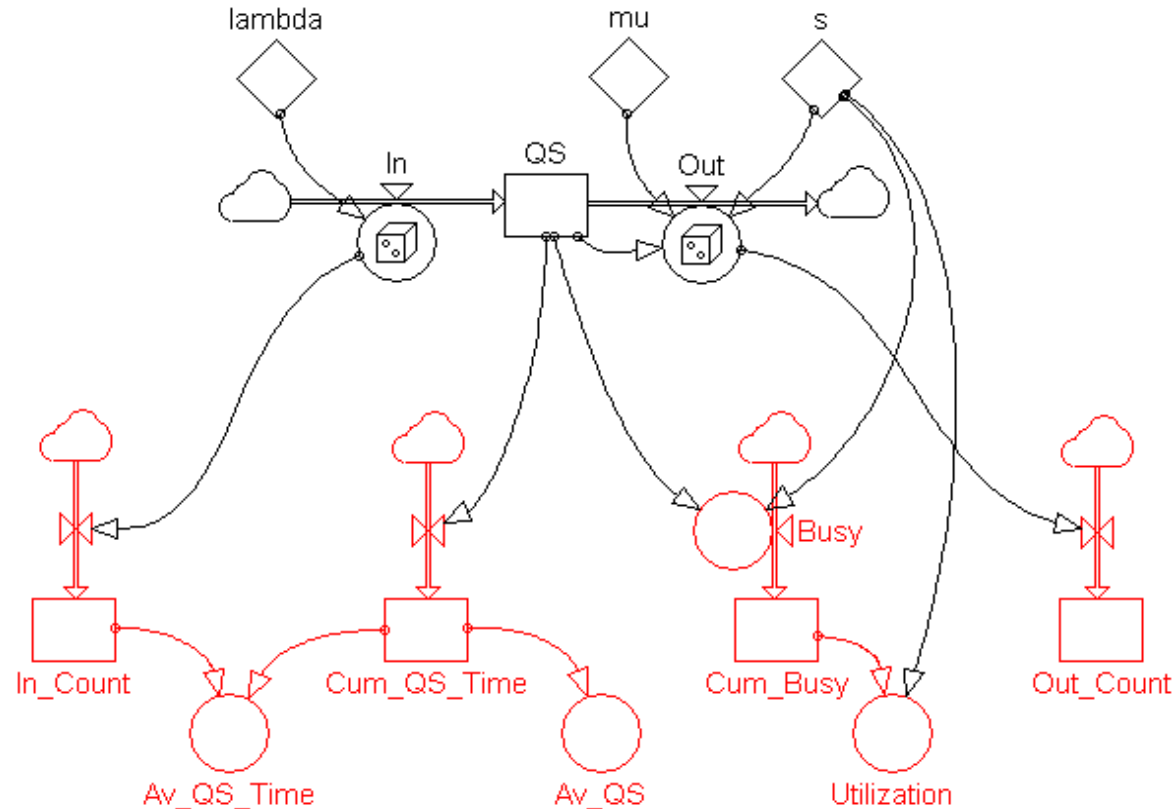
➔ Artefacts:



Stochastics must be modelled !
(Often can't just add or multiply random noise!)

- Non integer no. of atoms X
- X never levels out
- Variations never decrease
- The number of atoms may become negative
- When a quantity x_i becomes negative – equations including x_i may get mad and produce rubbish
- New atoms may be created
- Results depend on Δt
The shorter Δt the more energy in the noise.
- ...

Queuing systems are common in ABM & EBM. They can also be created in stochastic CBM (PoS)



An M/M/s queuing system. Here, QS is a compartment holding the total number of currently queuing and served tokens. The arrival rate is λ (*lambda*), the service rate (per server) is μ (*mu*) and the number of parallel servers is s .

The lower part of the diagram shows devices for counting arrivals and departures, and for calculating average queue-time, queue-length and server utilisation.

Warnings for deterministic compartment modelling

Be aware of the treacherous nature of deterministic modelling of populations.

Deterministic concepts force us to make a profound distortion of reality by:

- **replacing entities by continuous quantities** and
- **representing irregularly occurring events by smooth real-valued flows.**

Although this strongly simplifies the modelling, it often excludes a number of real aspects and phenomena and may create more or less biased results.

The modeller must be aware of the quagmire of potential problems. A deterministic model of a popul. must be tested against a corresponding stochastic population model.

A modellers should be very restrictive in the use of deterministic modelling of populations. Disciplines dealing with population models (ecology, epidemiology, etc.) should *not* base theories and studies on deterministic models.

- A deterministic model may behave very differently and produce wrong estimates.
- Neglecting stochastic jumps could change the mode of the solution: Real phenomena such as extinction or stochastically generated oscillations will get lost.
- All information about variations is lost: probability distribution functions, confidence intervals, extremes, correlations, etc.

Attractive properties of a (non-misleading) *deterministic* CBM

- + **If** average results are unbiased, then a deterministic model can produce the average results in just one simulation run (instead of averaging over many simulation runs of a stochastic model).
- + Parameter estimation, optimisation and sensitivity analysis are difficult and problematic to perform with stochastic models. If a deterministic model will reproduce average results correctly, then the deterministic model can be used to obtain estimates. These estimates can then be used in a corresponding stochastic model, which will reveal additional features such as the variability around the average outcomes.
- + A linear deterministic model is scalable – which is not the case for the corresponding stochastic model. You can then often simplify the modelling by working with fractions (instead of absolute numbers) of a population.

Situation-based modelling is extremely problematic

- + Mathematical calculation on the complete situation vector. Of theoretical value!
- Huge size already for relatively small models.
- Experience shows that the complexity often leads to over-simplification.
- The step-size (h) between points in time is implicit and fixed. (Change of h requires a total rebuilding of the transition matrix.)
- Any model change requires a complete rebuilding of \mathbf{P} .
- Time varying parameters or environmental stochasticity requires rebuilding the transition matrix each time step.
- Bad structural overview.
- Execution time is long.
- Model fitting is very problematic.
- Etc.

(NOTE that the underlying *conditional probability* $[P(A|B)]$ and the Markov condition (memorylessness) are *not* unique for Markov models. They are equally true for ABM, EBM and CBM .)

Decomposing a model into situations will only create problems without giving any advantage in simulation! Stay away from situation-based models in simulation!