

Introduction to Modelling and Simulation

Methods and Algorithms

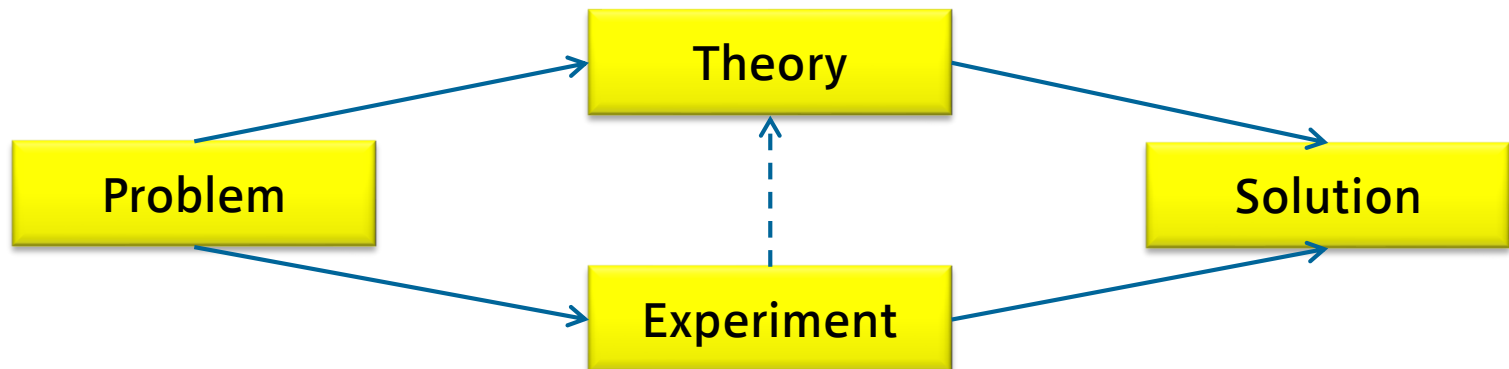
Classical Scientific Problem

- Application of Theories
- Execute Experiments



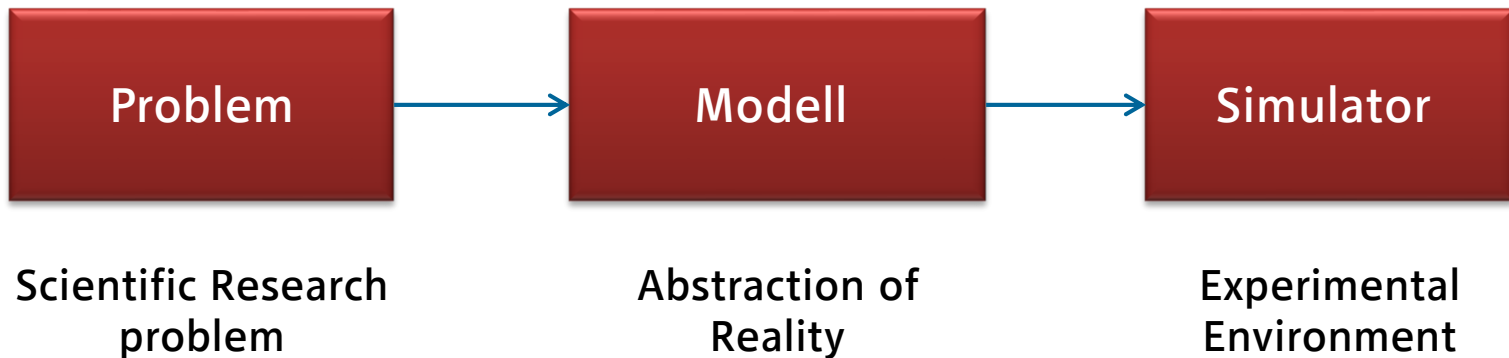
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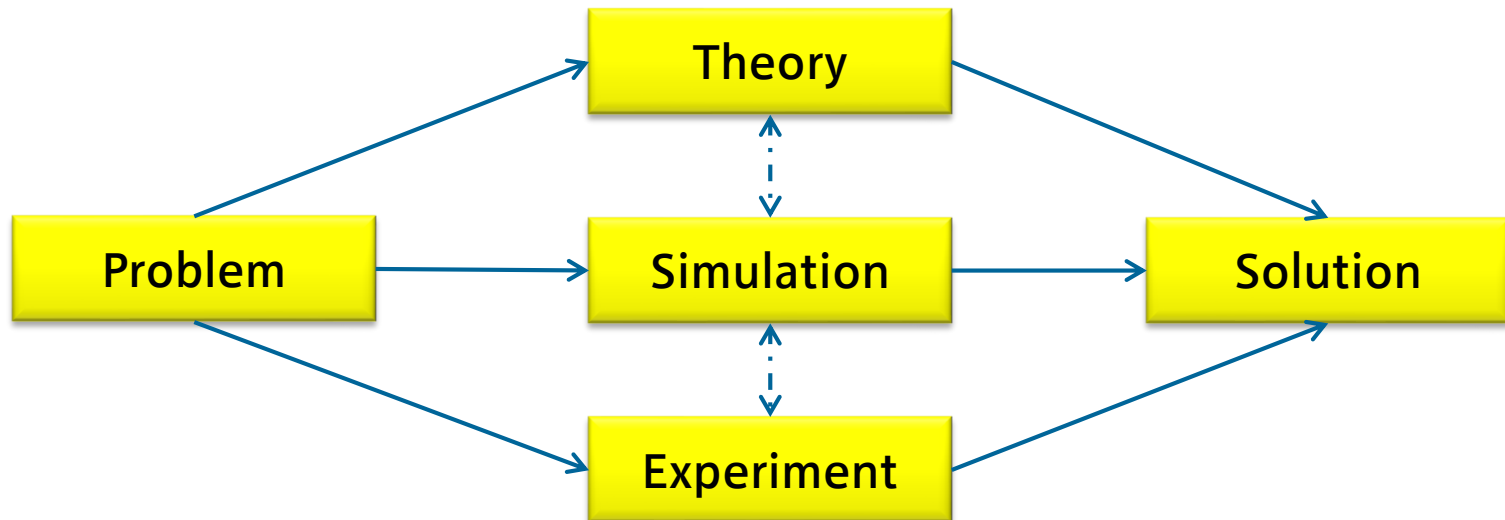
Simulation

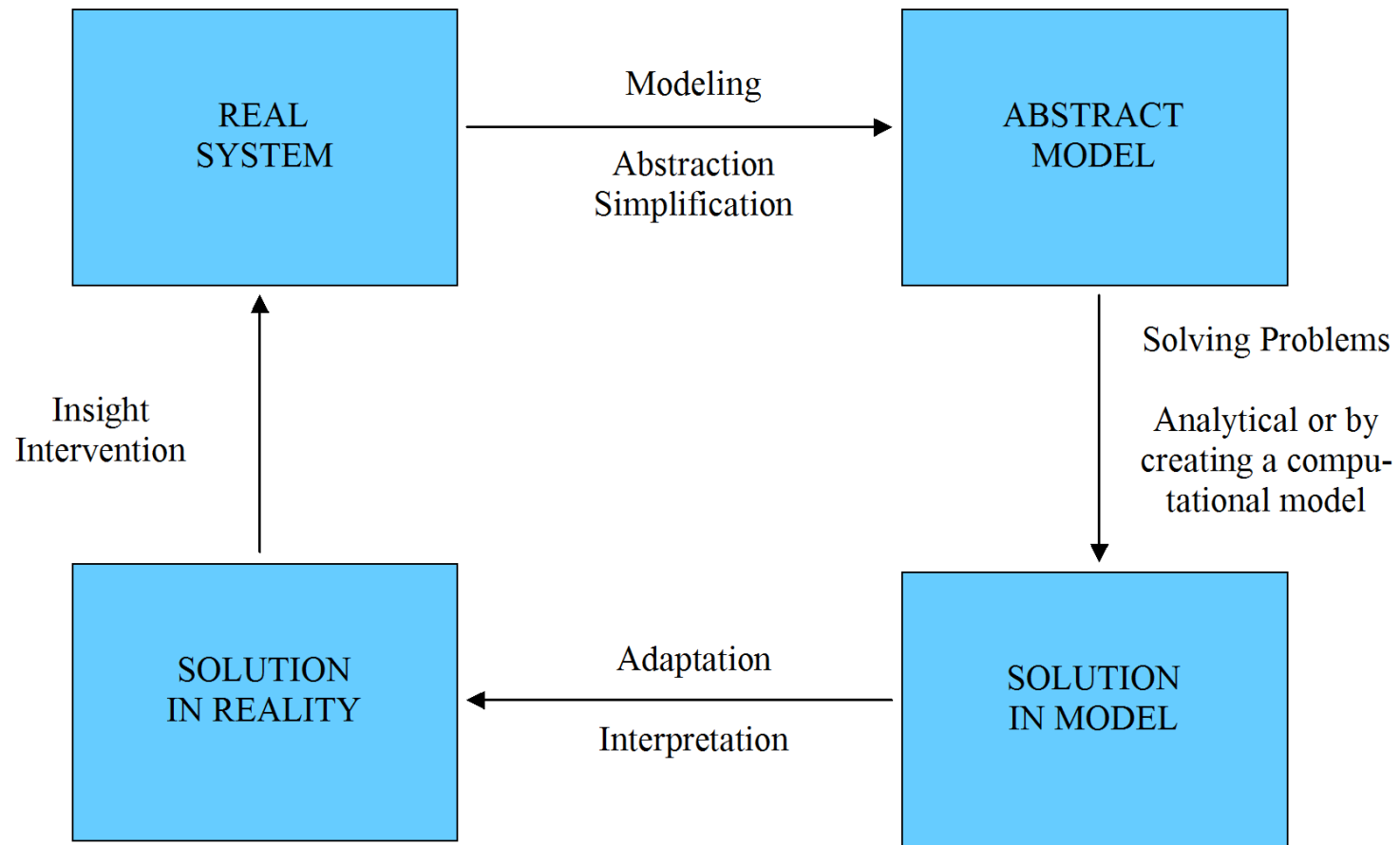
- Experiments in virtual laboratory
- Experiments in the computer
- The third pillar of science beside theory and experiment



Simulation

- Experiments in virtual laboratory
- Experiments in the computer
- The third pillar of science beside theory and experiment





Definition (Shannon, 1975)

Simulation is the process of designing a **model** of a real system and conducting **experiments** with this model for the **purpose** either of **understanding the behavior** of the system and its underlying causes or of **evaluating various designs** of an artificial system or **strategies for the operation** of the system.

Definition 2 (VDI-Richtlinie 3633)

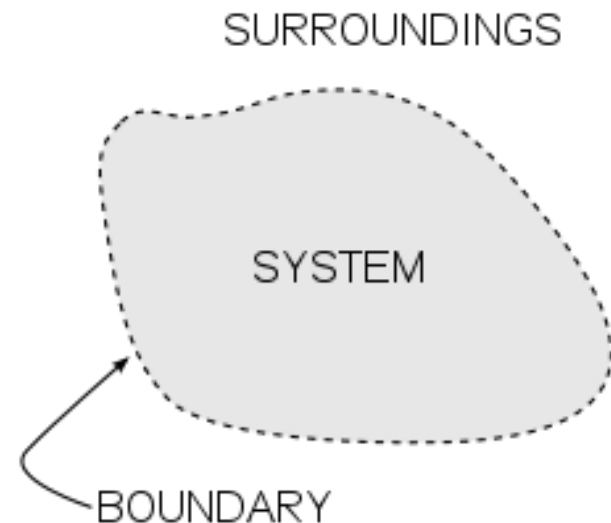
Simulation is a (virtual) **copy of a real system** with its dynamic processes in a (virtual) model (**computer model**) and (virtual) experiments with **experiments** with this model, which allow **interpretations** for the real system.

In a practical sense, **simulation** is i) **preparing**, ii) **performing**, and iii) **evaluating experiments** with a simulation **model**.

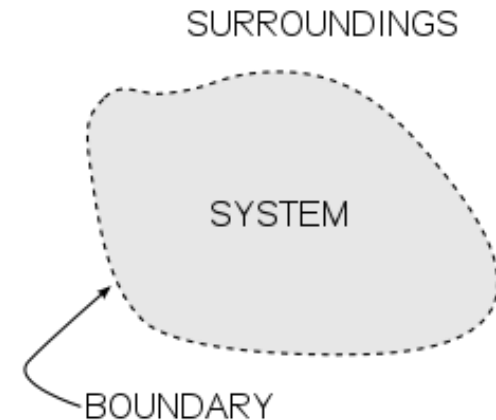
Simulation allows to study **time-dependent behaviour** of **complex dynamical systems** in a simulation **model**.

A **system** is a set of interacting or interdependent components forming an **integrated whole**

A **dynamic system** is a set of **dynamically interacting or interdependent components** forming an **integrated whole**

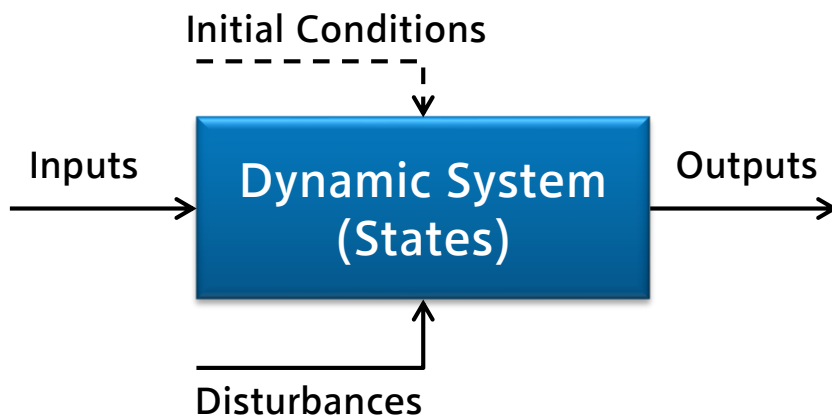
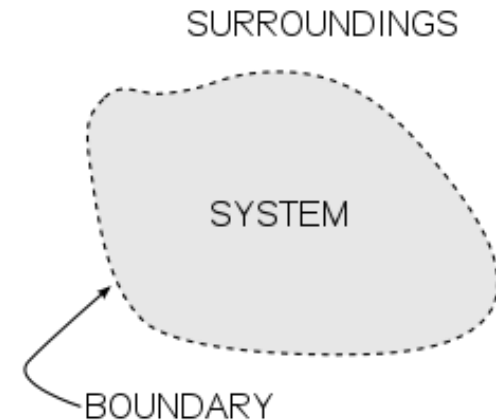


A **dynamic system** is a set of **dynamically interacting or interdependent components** forming an **integrated whole**



- **Dynamical systems** change their **behaviour dependent on acting input signals**, disturbances, and initial values
-
- The **behaviour of a dynamical system** is not direct proportional to input and disturbance change, it **changes** its behaviour **on basis of its own dynamic** and on inputs.

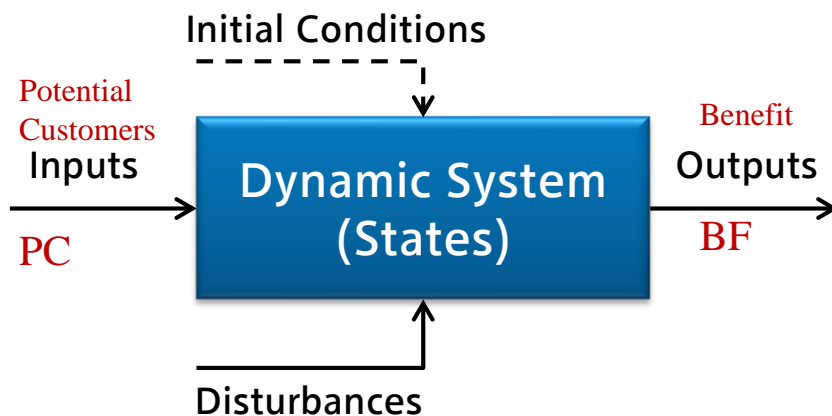
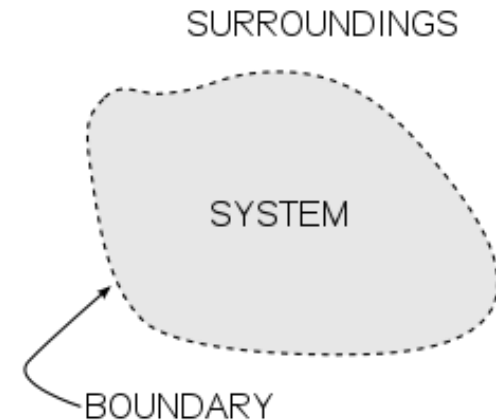
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Elements of a Dynamical System

- States $x(t)$
- Inputs $u(t)$
- Disturbances $w(t)$ = Inputs
- Outputs $y(t)$
- Fixed Parameters, Initial Conditions
- Time dependent Parameters (Inputs)

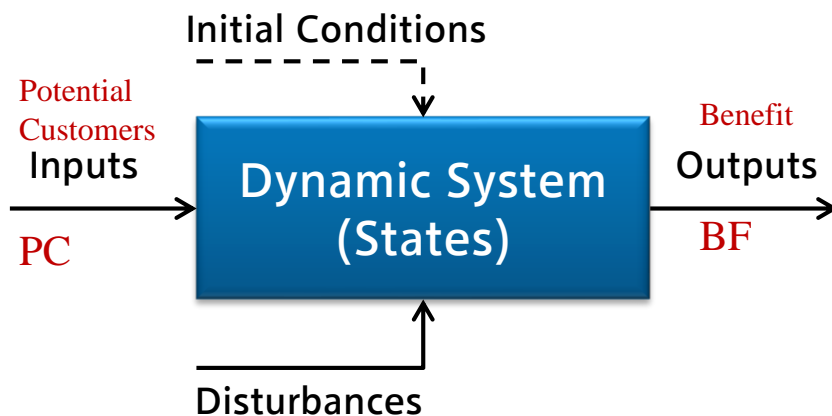
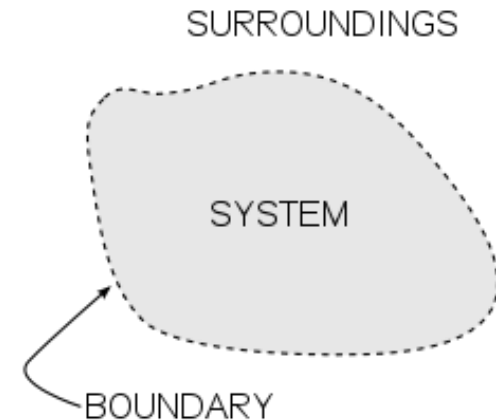
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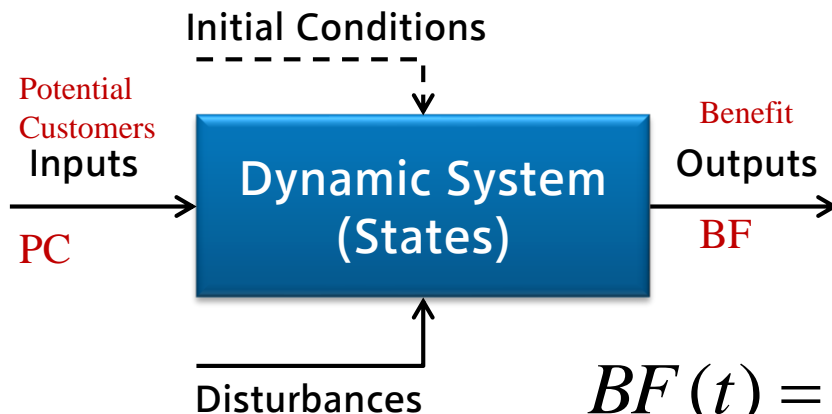
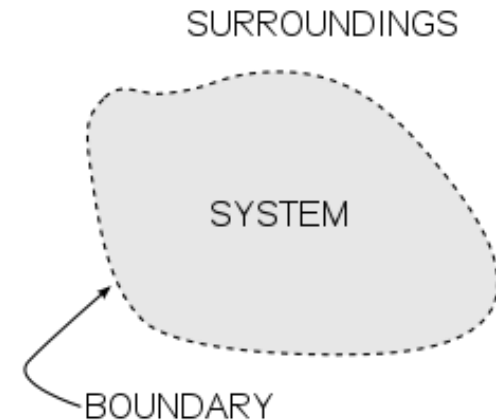
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static

$$BF = Faktor \cdot PC$$

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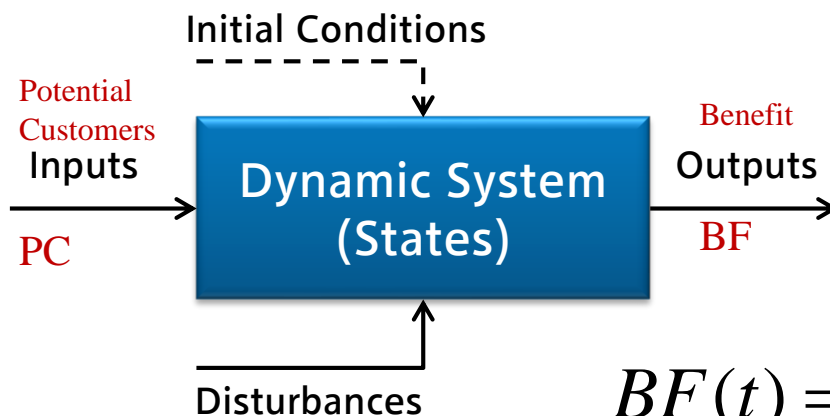
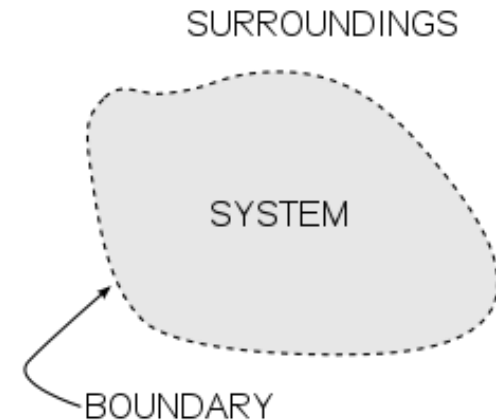
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dynamic

$$BF(t) = Function(PC(t), t, Parameters)$$

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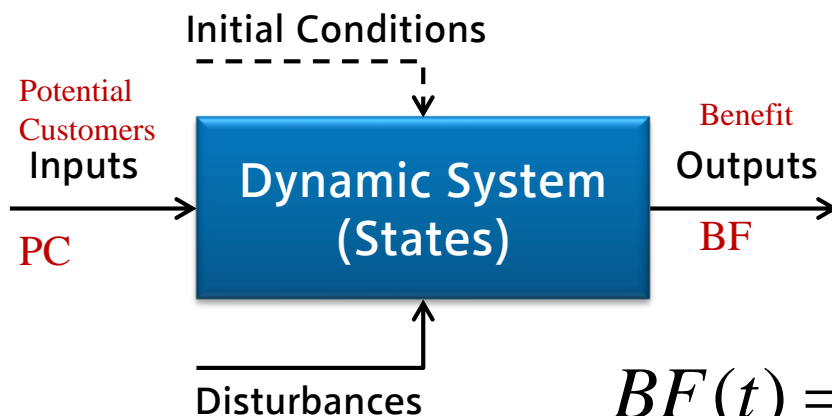
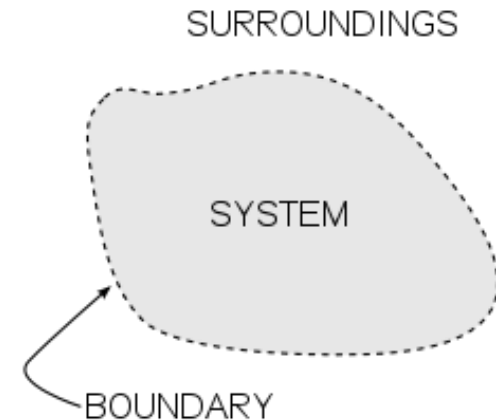
static

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really dynamic

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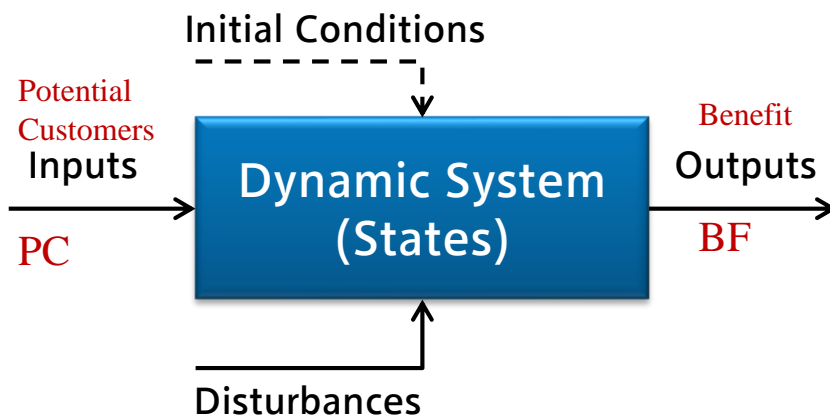


static formula

$$BF = Faktor \cdot PC$$

dynamic model

$$BF(t) = Function(PC(t), BF(t), t, Par)$$



static formula

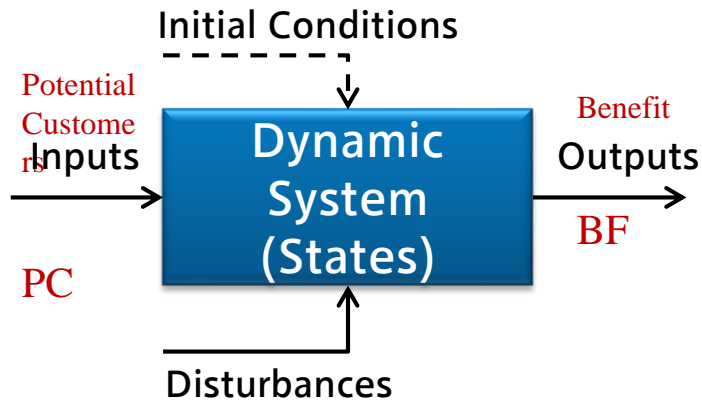
$$BF = Faktor \cdot PC$$

Calculation

dynamic model

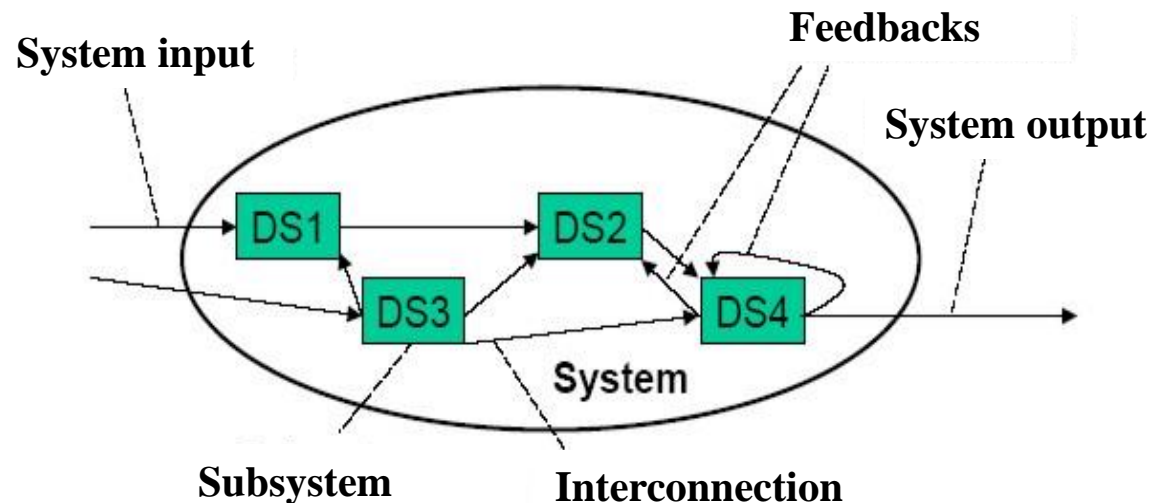
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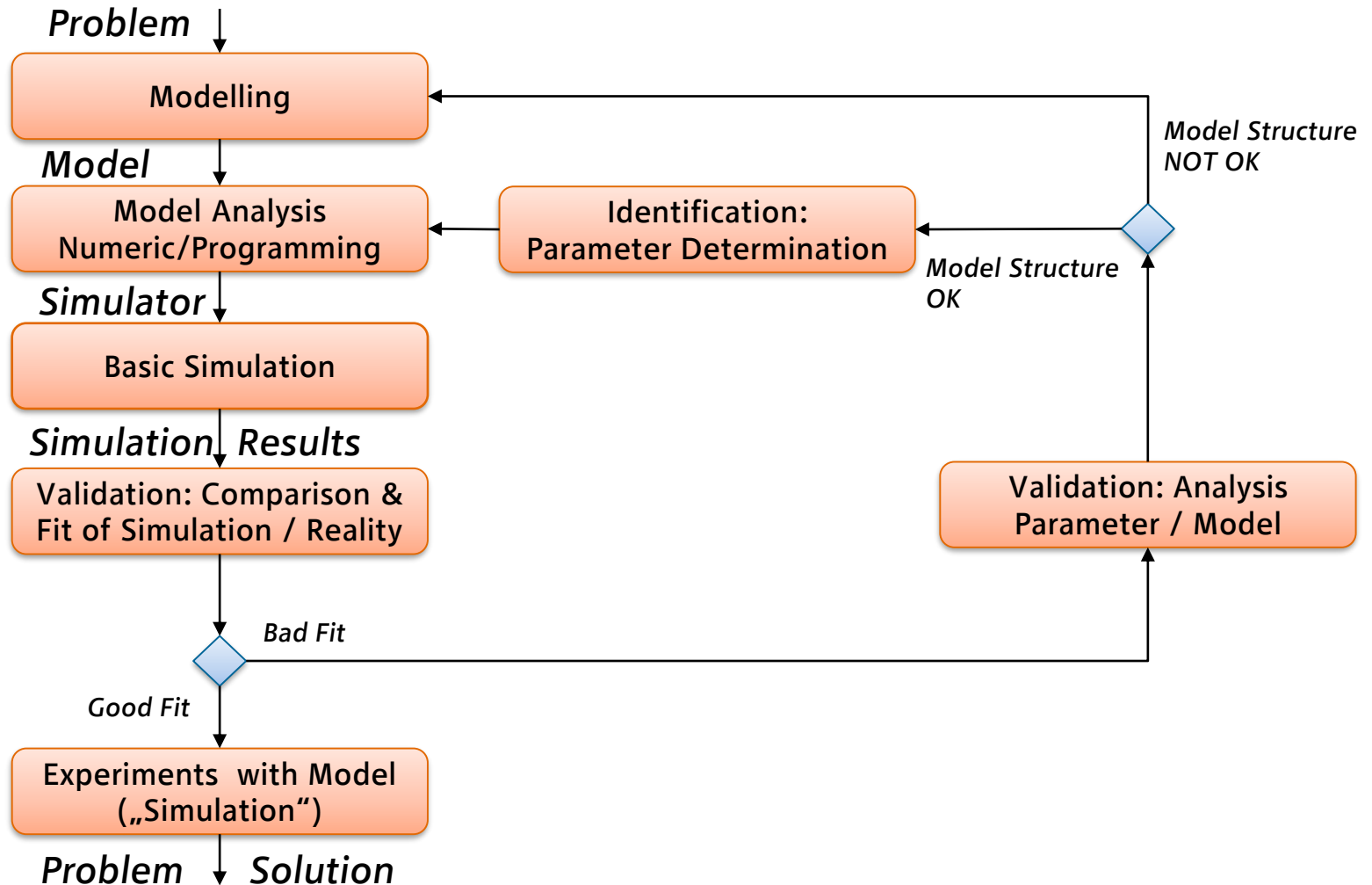
Simulation

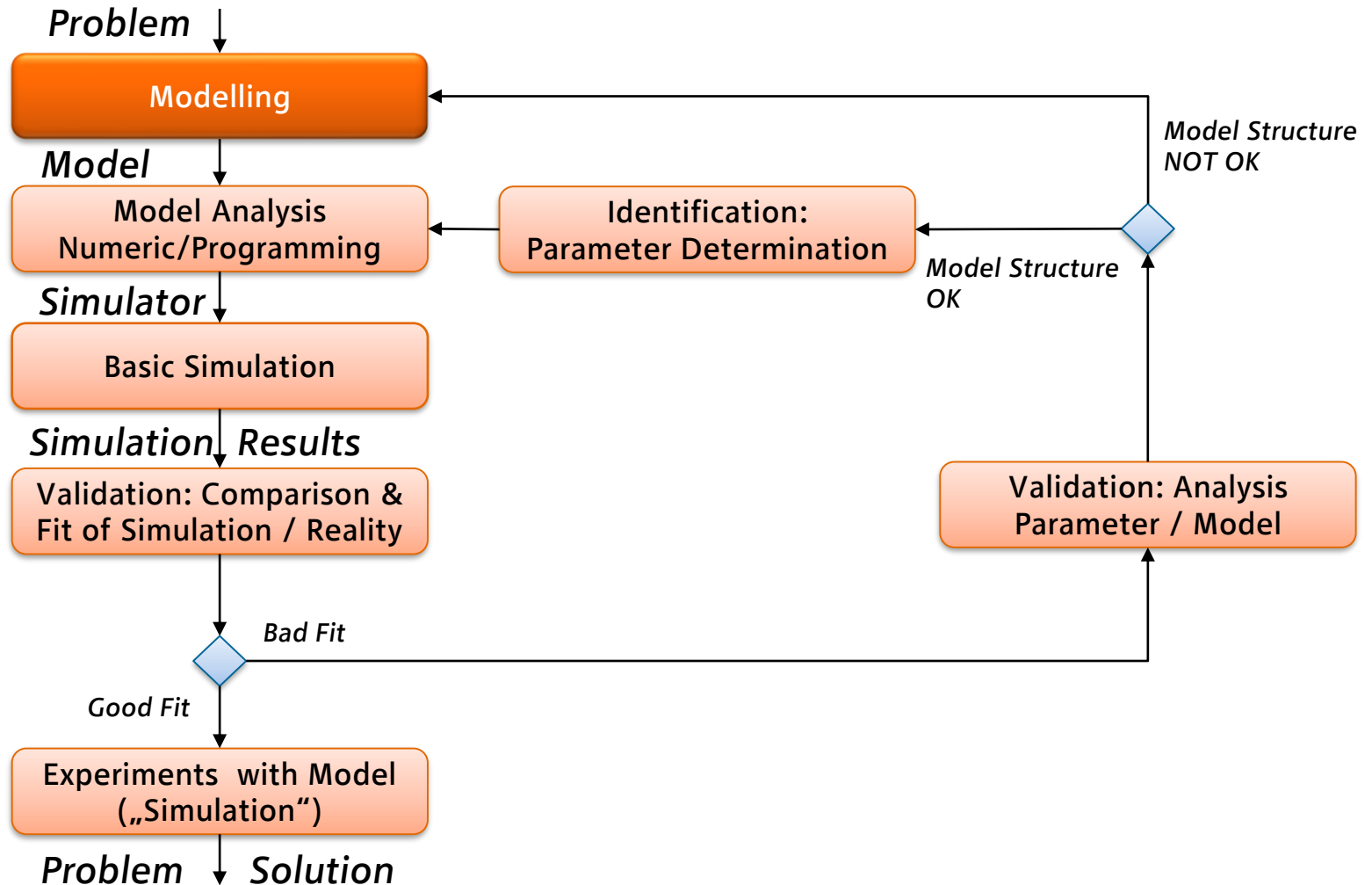


Dynamic mathematical model
 $BF(t) = \text{Function}(PC(t), BF(t), t, par)$
Simulation

A **dynamical system** may consist of a **set of components**, which themselves are **dynamical subsystems** and which **influence each other**



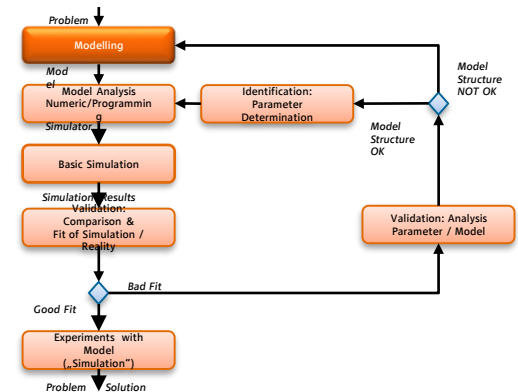


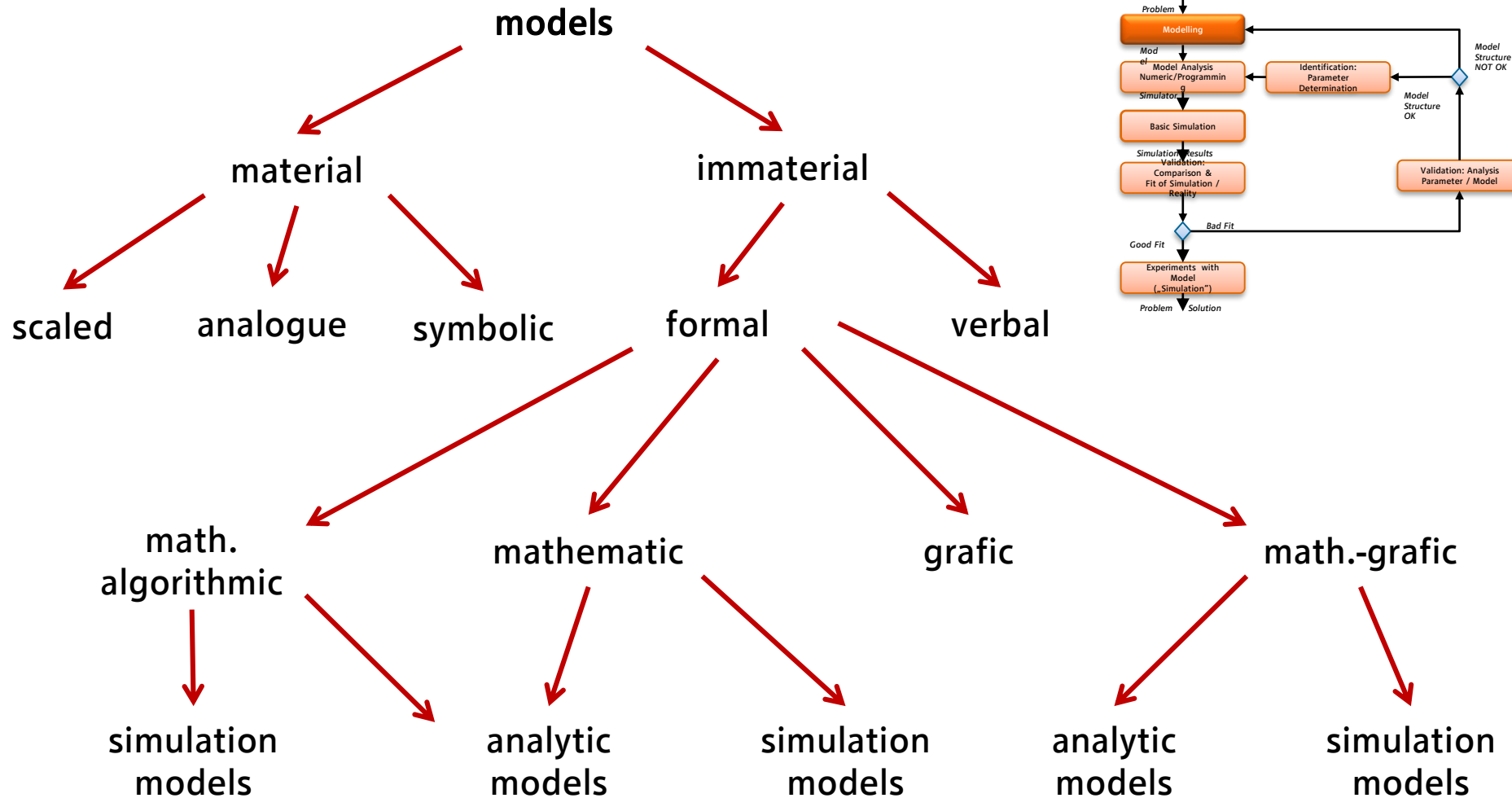


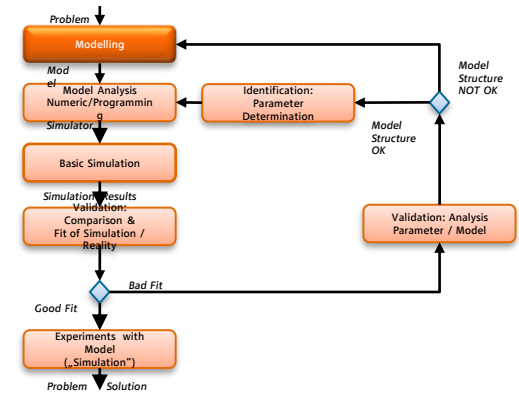
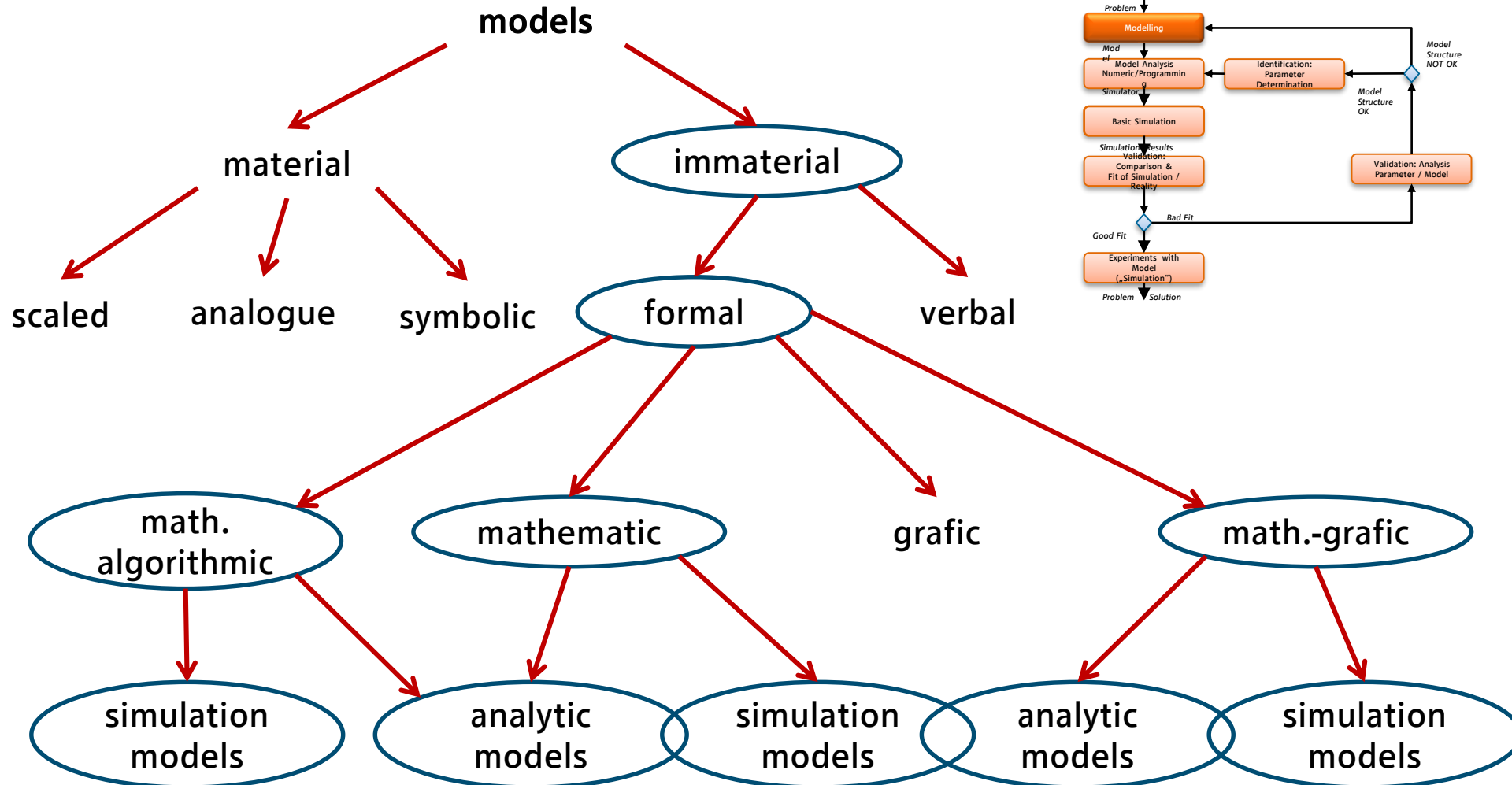
What is a Model?

1. **Mapping** - A model is a representation of a natural or an artificial object.
2. **Reduction** - A model is usually simplified and does not have all attributes of the original object.
3. **Pragmatism** - A model is always created for a certain purpose, a certain subject and a certain time-span.

(Stachoviak 1973)







Two Steps of Abstraction

- **Structural Abstraction** – Qualitative Knowledge
Identification of system borders and states
- **Phenomenological Abstraction** – Quantitative Knowledge
quantisation of states, identification of physical, economic, biologic, ... interactions in and with subsystems

Modelling Approach

- System Dynamics (SD)
- Transfer Functions (TF)
- Compartment Modelling
- Math. Formula
- Lagrange Formalism
- Port-based physical Modelling
- Difference Equation Modelling
- Cellular Automata Modelling
- Agent-based Modelling
- Event Graphs
- Process Flow

Model Type

- Ordinary Differential Equations (ODEs)
- Partial Differential Equations (PDEs)
- Differential Algebraic Equations (DAEs)
- Difference Equations (DEs)
- Cellular Automata (CAs)
- Agent-based Systems/Models (ABMs)
- Discrete Event Systems (DES)

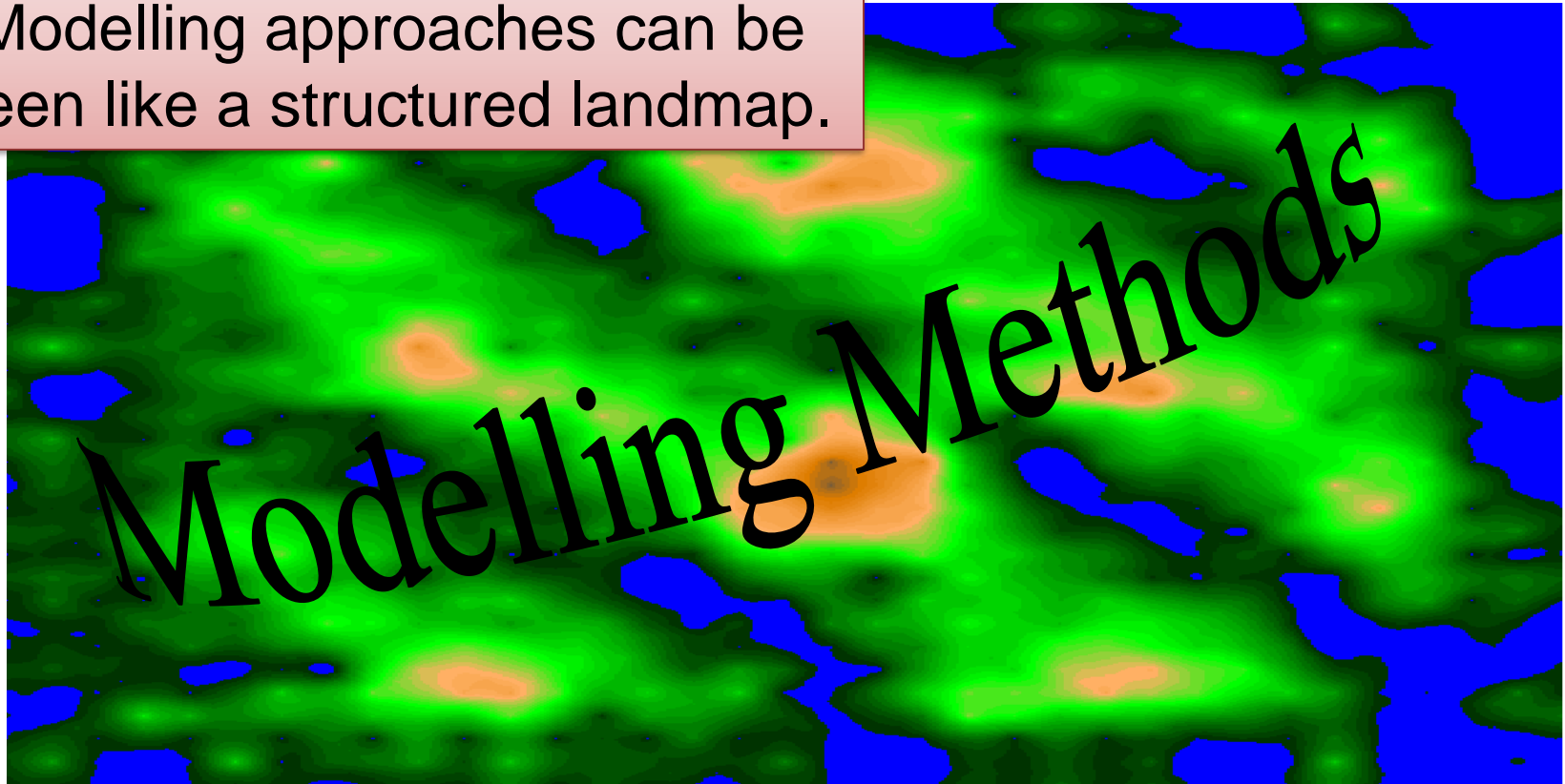
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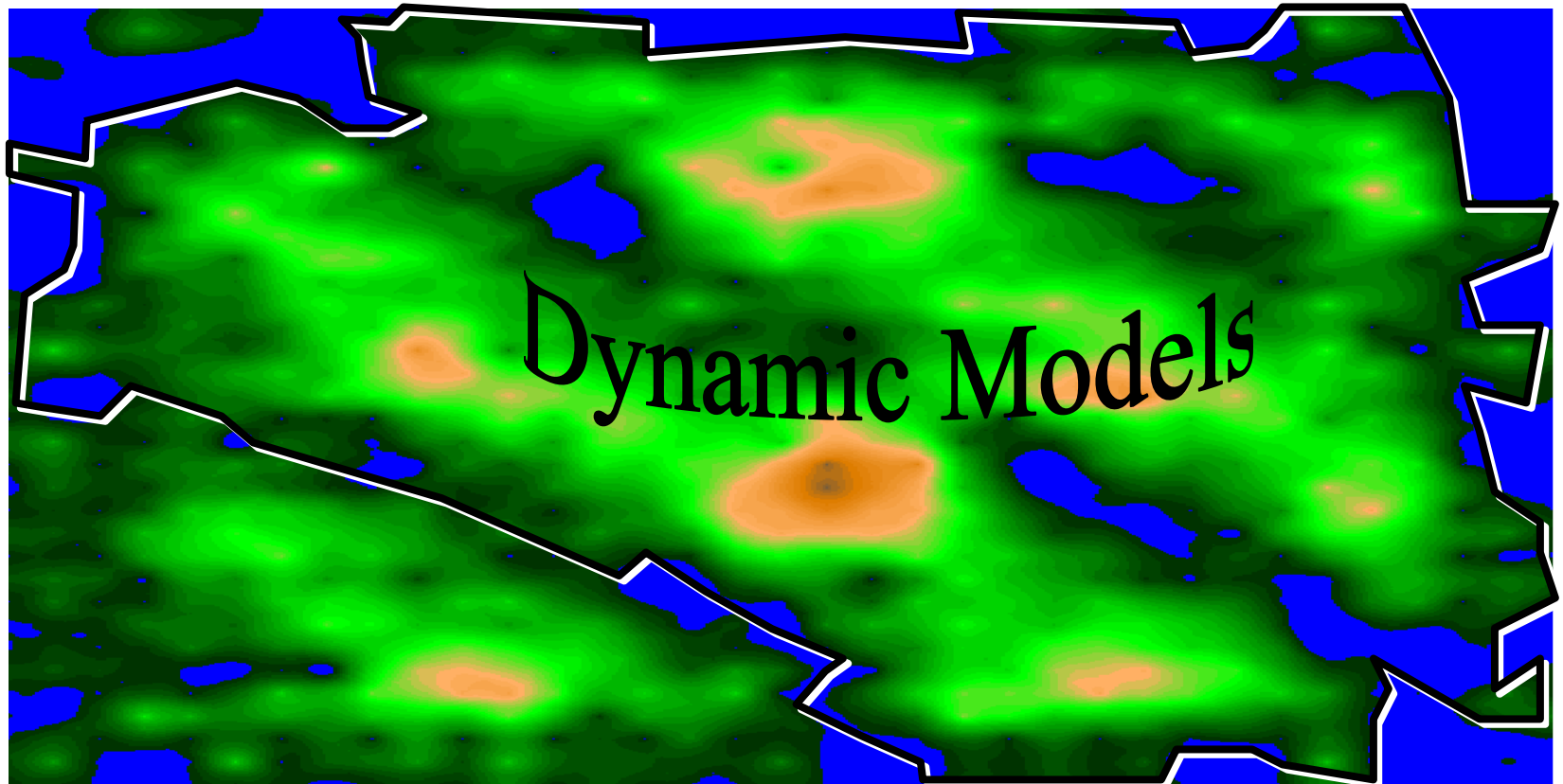
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The variety of different Modelling approaches can be seen like a structured landmap.



Landmap of Modelling Methods – Dynamic Models

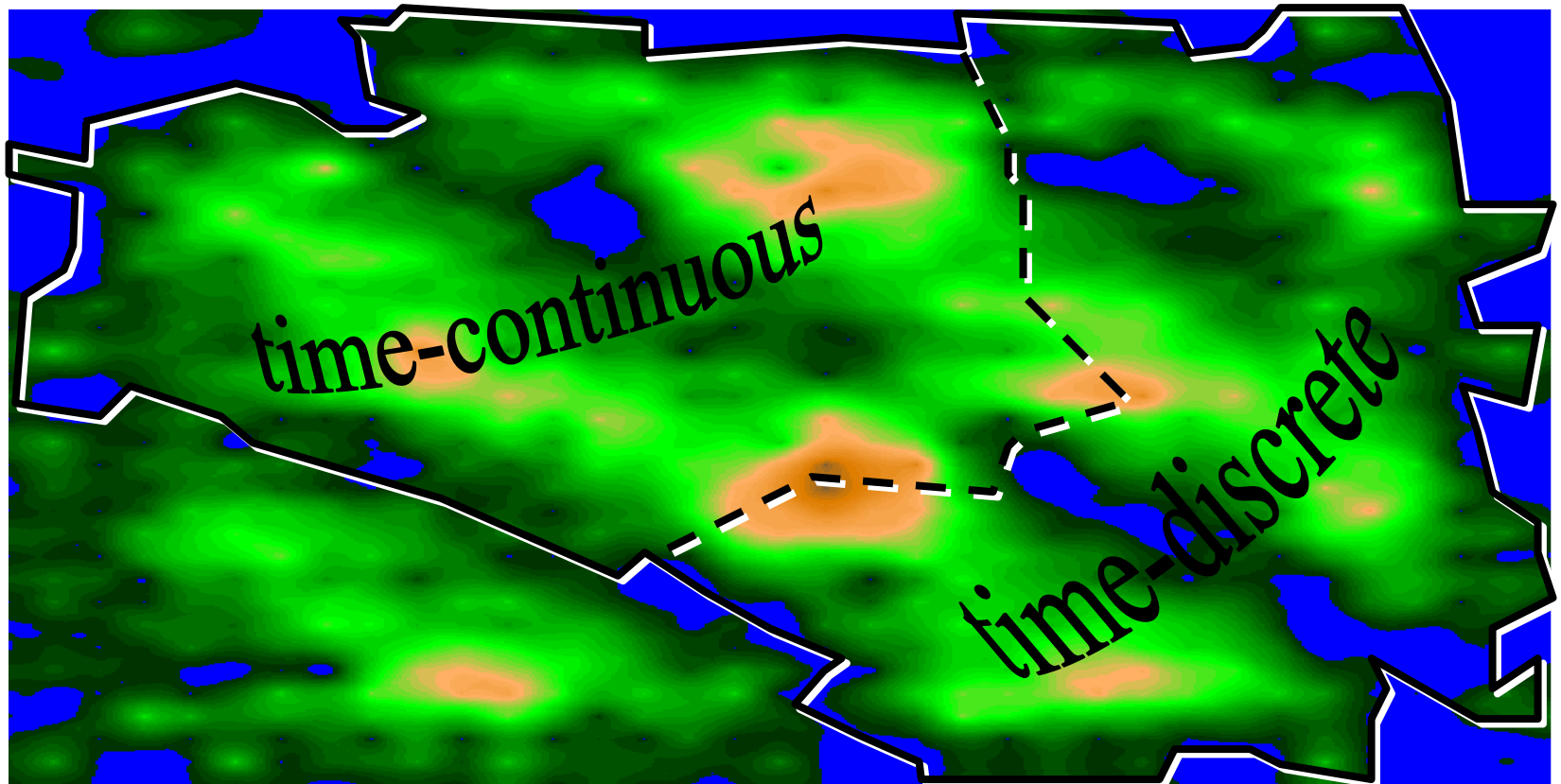


Neglecting quantum-mechanics (space as well as) time can be seen to be a continuous number.

- A model is called **time-continuous** if the output value of the model can be calculated at **any time** ($\approx t \in \mathbb{R}$).
- In the opposite a model is called **time-discrete** if values are only calculated at a finite number of predefined **timesteps** ($\approx t \in \mathbb{N}$).

- Usually time-continuous models are preferred to time-discrete models, but the simulation process is usually more difficult.
- Yet, there are processes in real world for which time continuous models are not necessary or even don't make sense.
- Very often, time-continuous models cannot be **simulated** continuously. So they need to be reformalised in a time-discrete manner – this process is called **discretisation**.

Landmap of Modelling Methods – Time Discrete / Continuous



Similar to time-discrete/continuous, also output values can be determined discrete or continuously.

- **Value-discrete:**
 - Number of passengers on a plane
 - Number of cars searching for a parking spot.
- **Value-continuous:**
 - Voltage/Current in an Electrical Circuit
 - Angular Velocity of a Pendulum

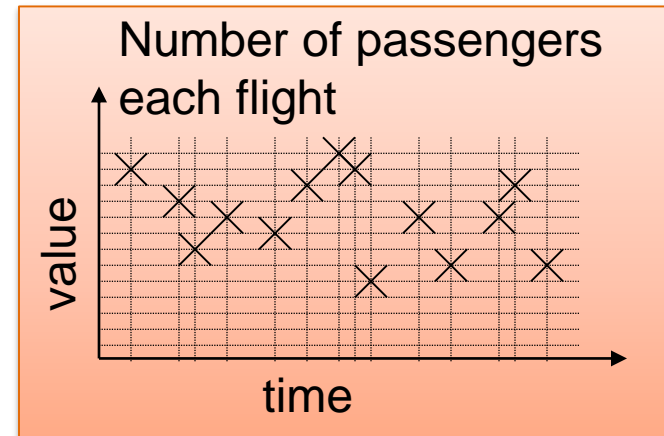
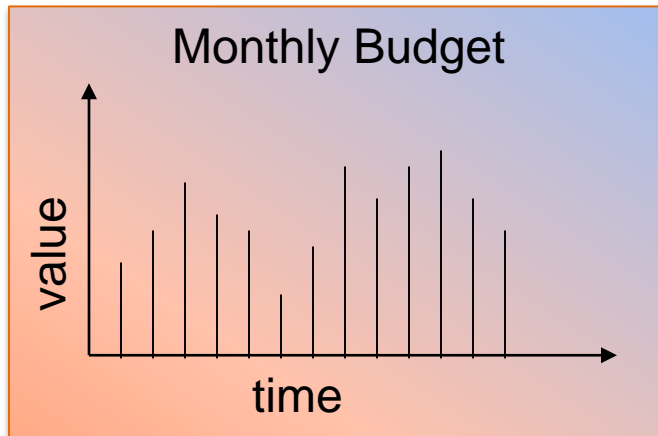
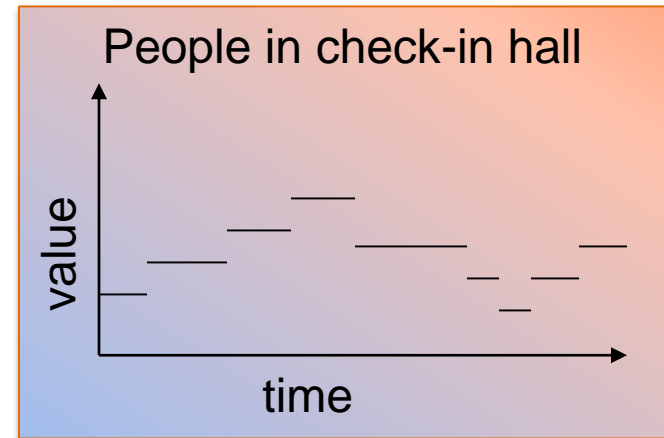
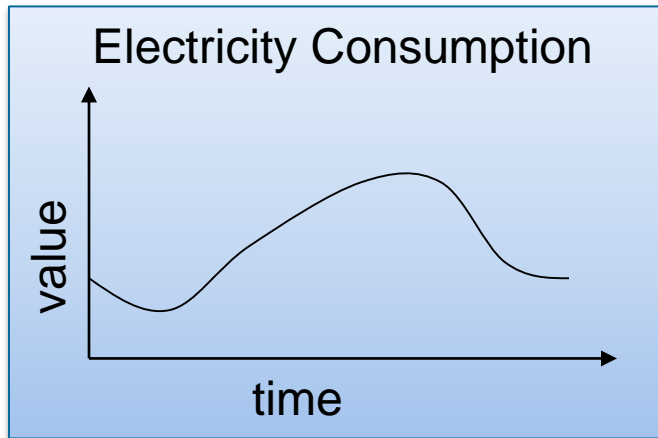
- Although simulation output is expected to be continuous/discrete, it is **not necessarily modelled** in a continuous/discrete way.

E.g.:

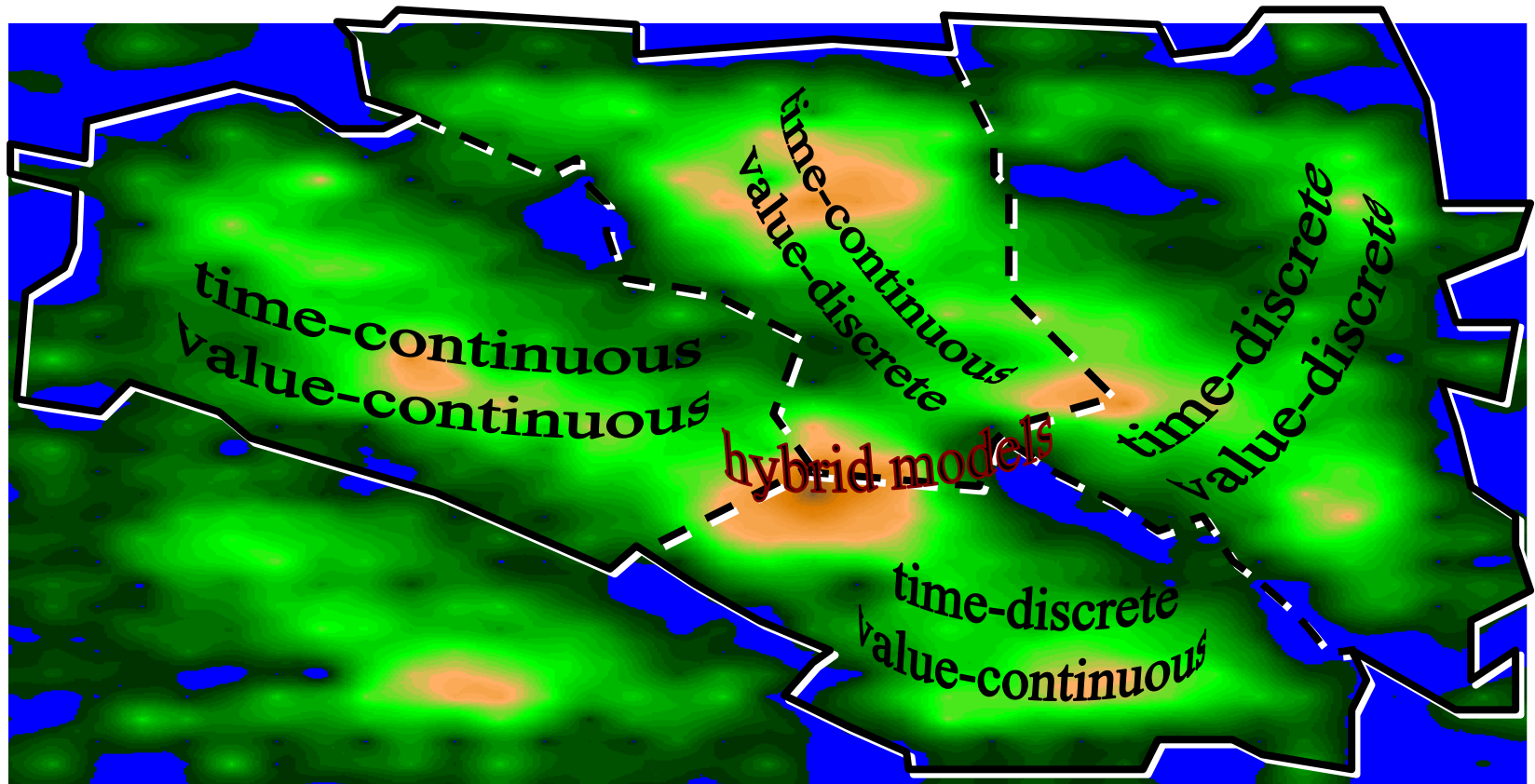
*Population of a country is a discrete number...
... yet it can be modelled by a continuous
model*

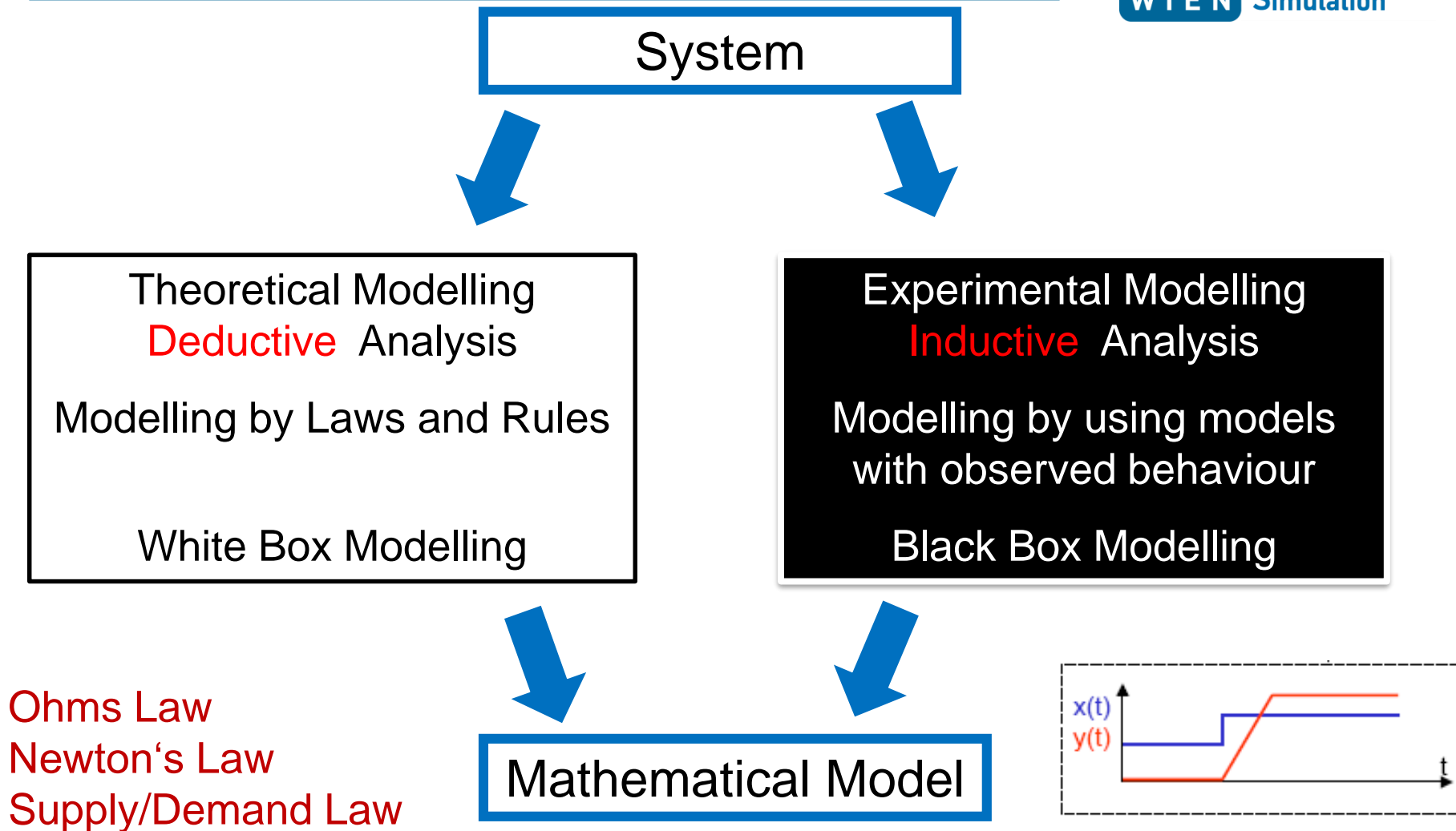
It requires a correct result interpretation!

Examples –Discrete/Continuous



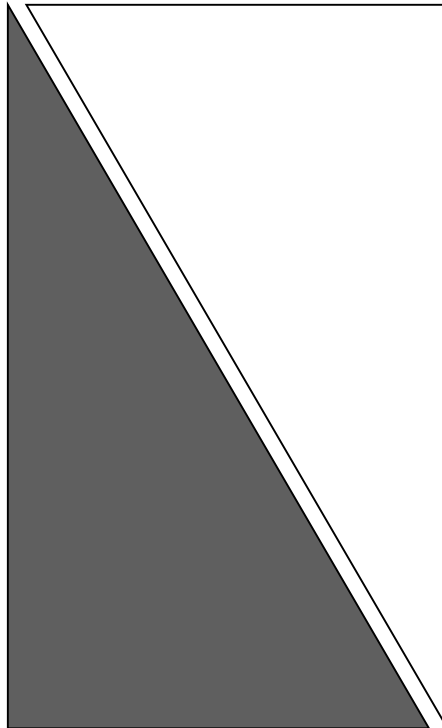
Landmap of Modelling Methods – Discrete / Continuous





White Box Modeling

- Electrotechnique
- Mechanics
- Environment
- Medicine
- Economy
- Sociology

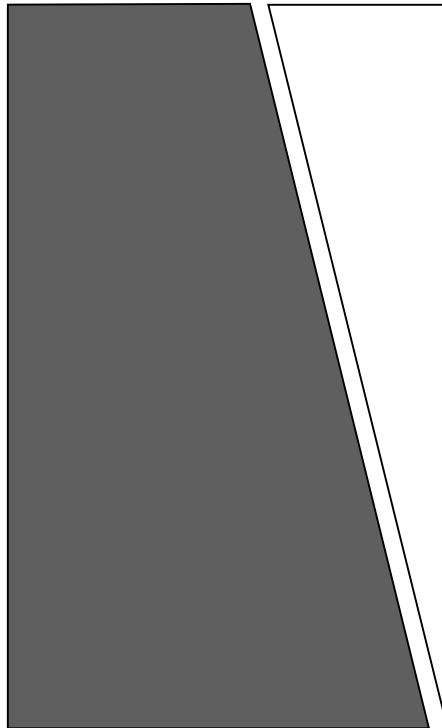


- Laws
- Laws and Observations
- Laws and Observations
- Observations and Characterisation
- Observations and Characterisation

Black Box Modeling

From Deduction to Induction

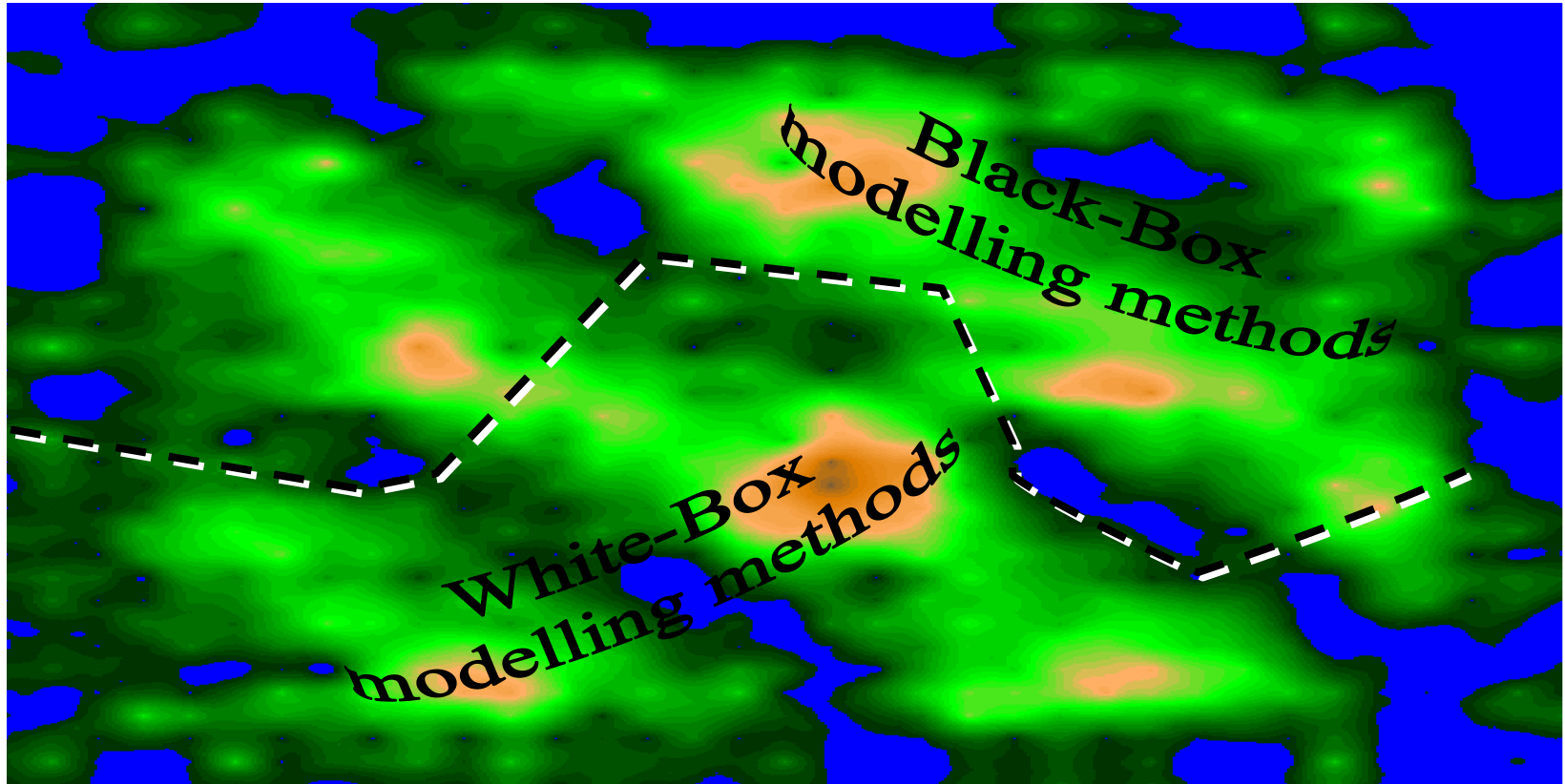
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Deductive models may contain too many parameters –
problems with identification

Landmap of Modelling Methods – Discrete / Continuous



- If the output of the simulation of a model is uniquely defined by input parameters, initial conditions and model parameters the model is called **deterministic**.
- Otherwise it is called **stochastic**.



⇒ deterministic



⇒ stochastic

Stochastic models are necessary...

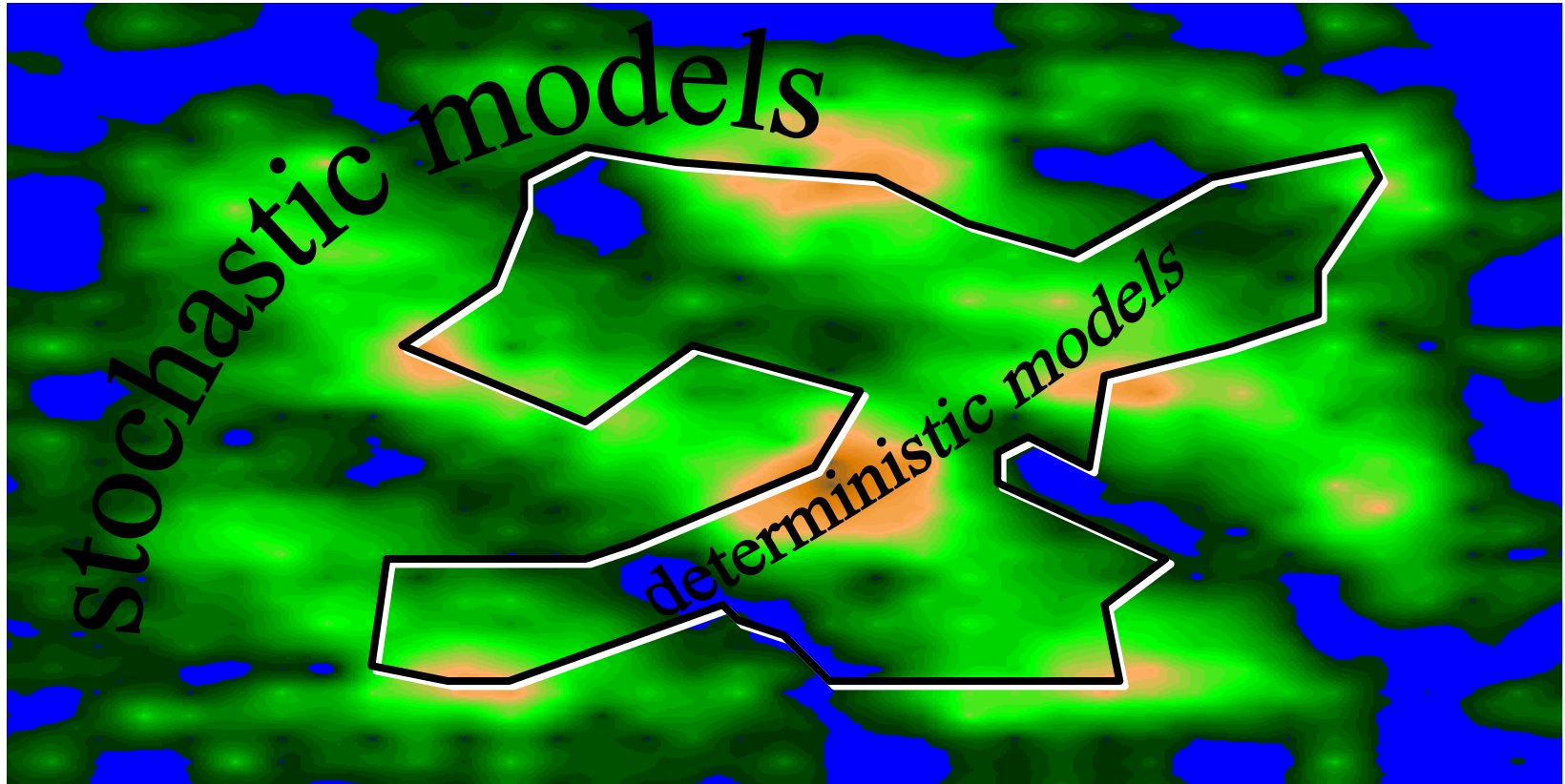
- ... if random effects are included in the system.
→ coin toss, rolling a dice, ...
- ... if elements of the system are too complex to be described by deterministic rules.
→ human behaviour, problems at system borders,...

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Landmap of Modelling Methods – Discrete / Continuous

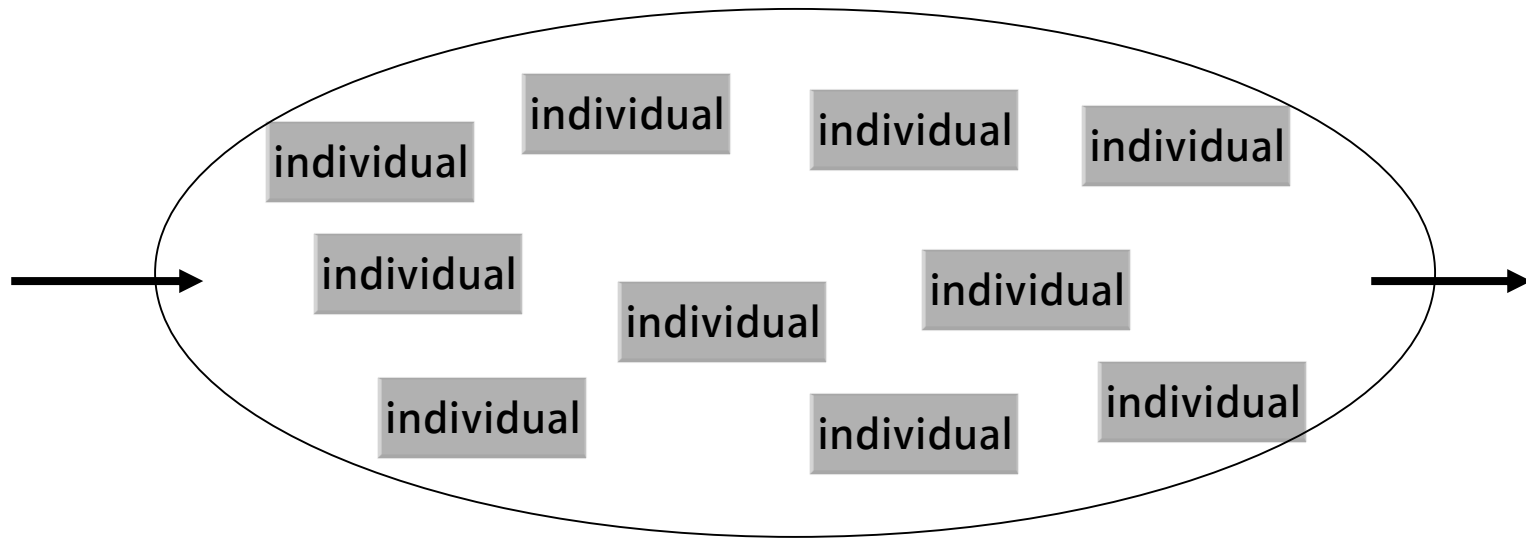


- If systems consist of a big set of similar subsystems...

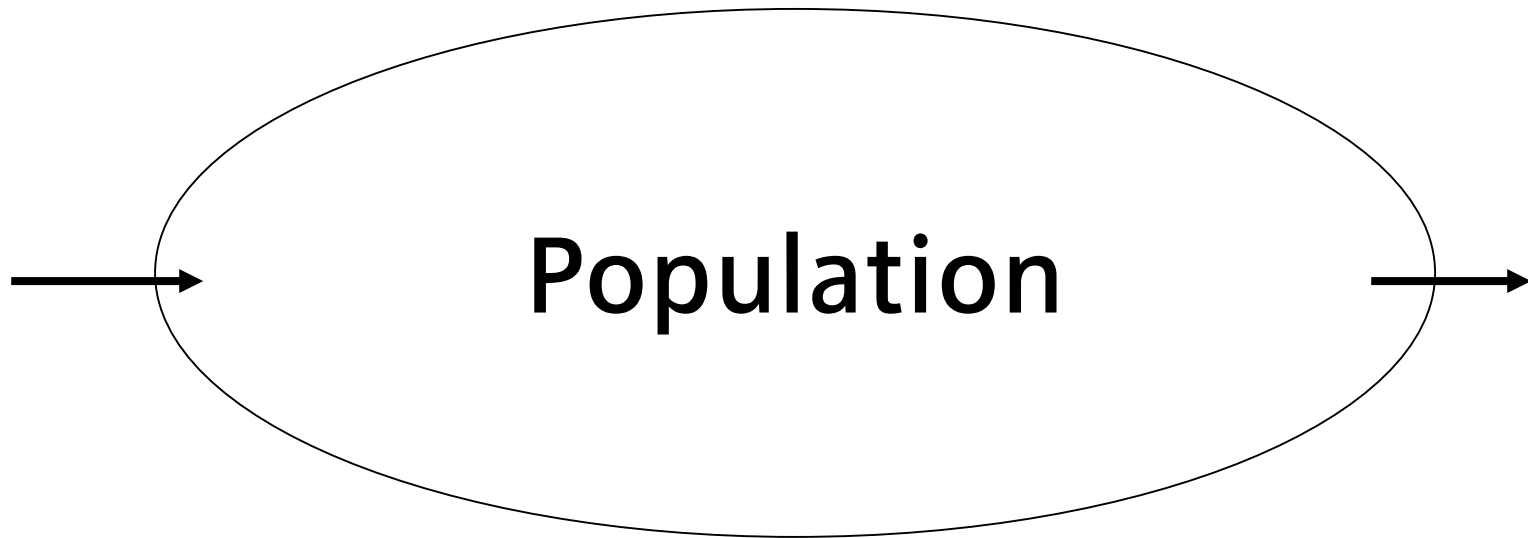
Population	individual
Company	subsidiary
Traffic	car
Paper	wooden fibre

... the question arises whether a micro- meso- or macroscopic model should be used.

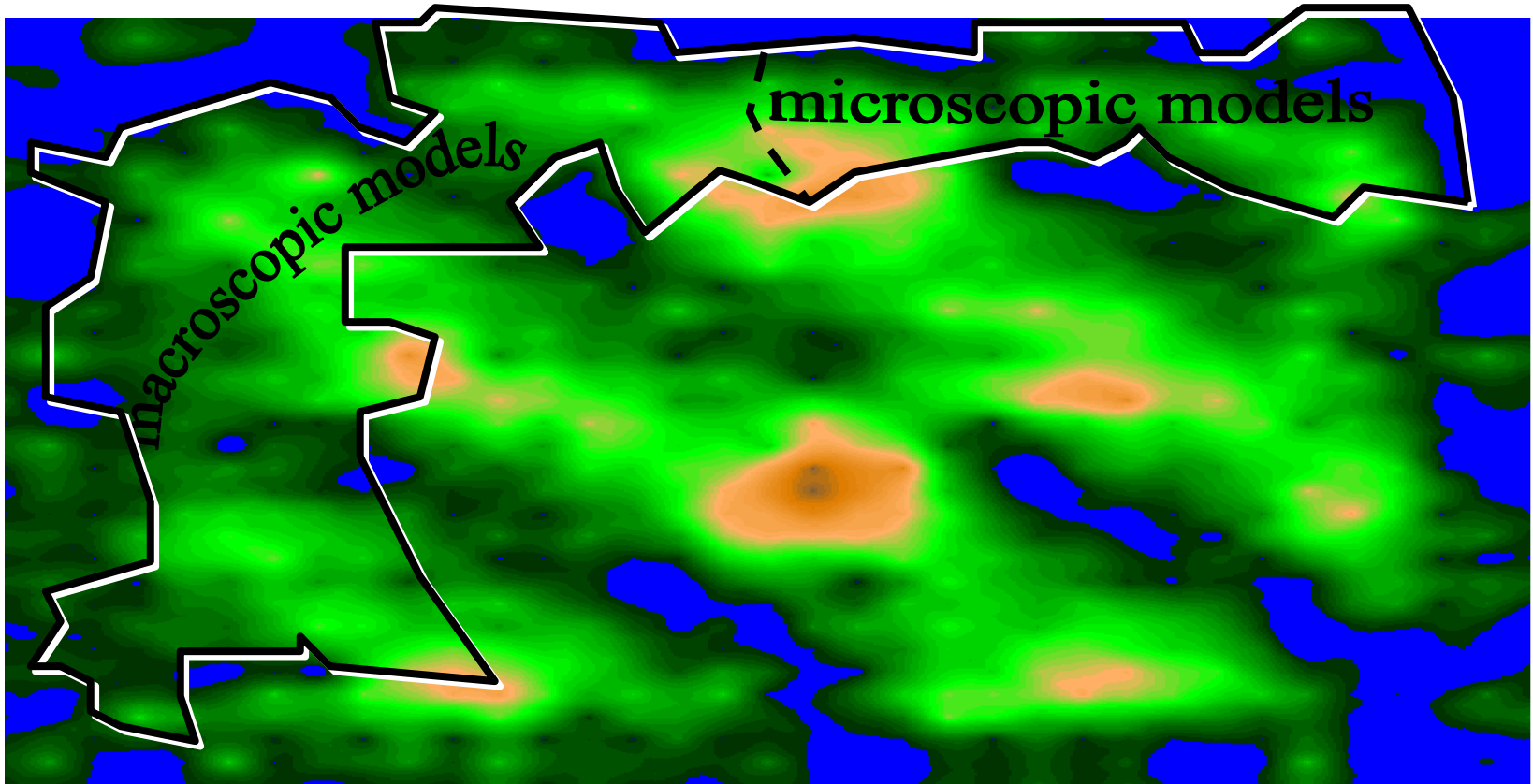
- Microscopic models treat each subsystem as an individual model. Finally they are linked in order to model the whole system.



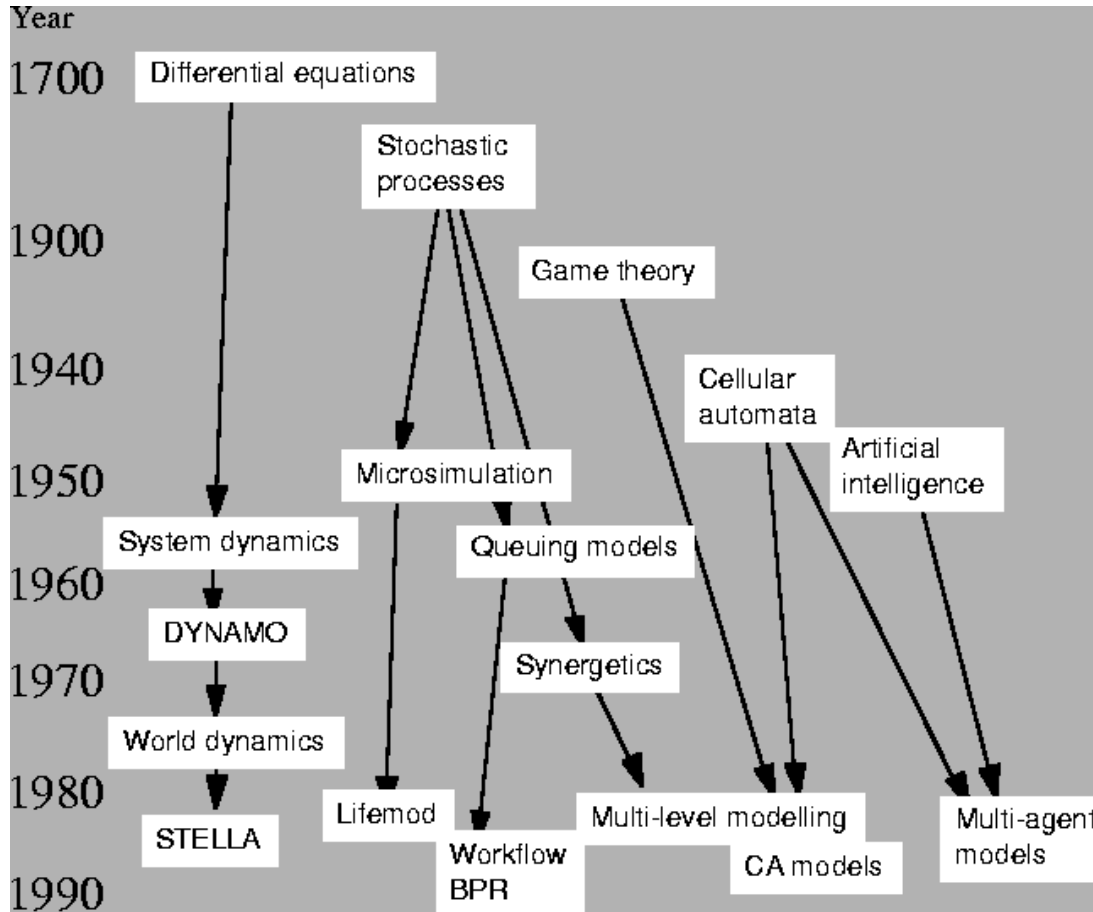
- Macroscopic models treat the whole system, neglecting the fact, that it consists of subsystems.



Landmap of Modelling Methods – Microscopic/Macroscopic

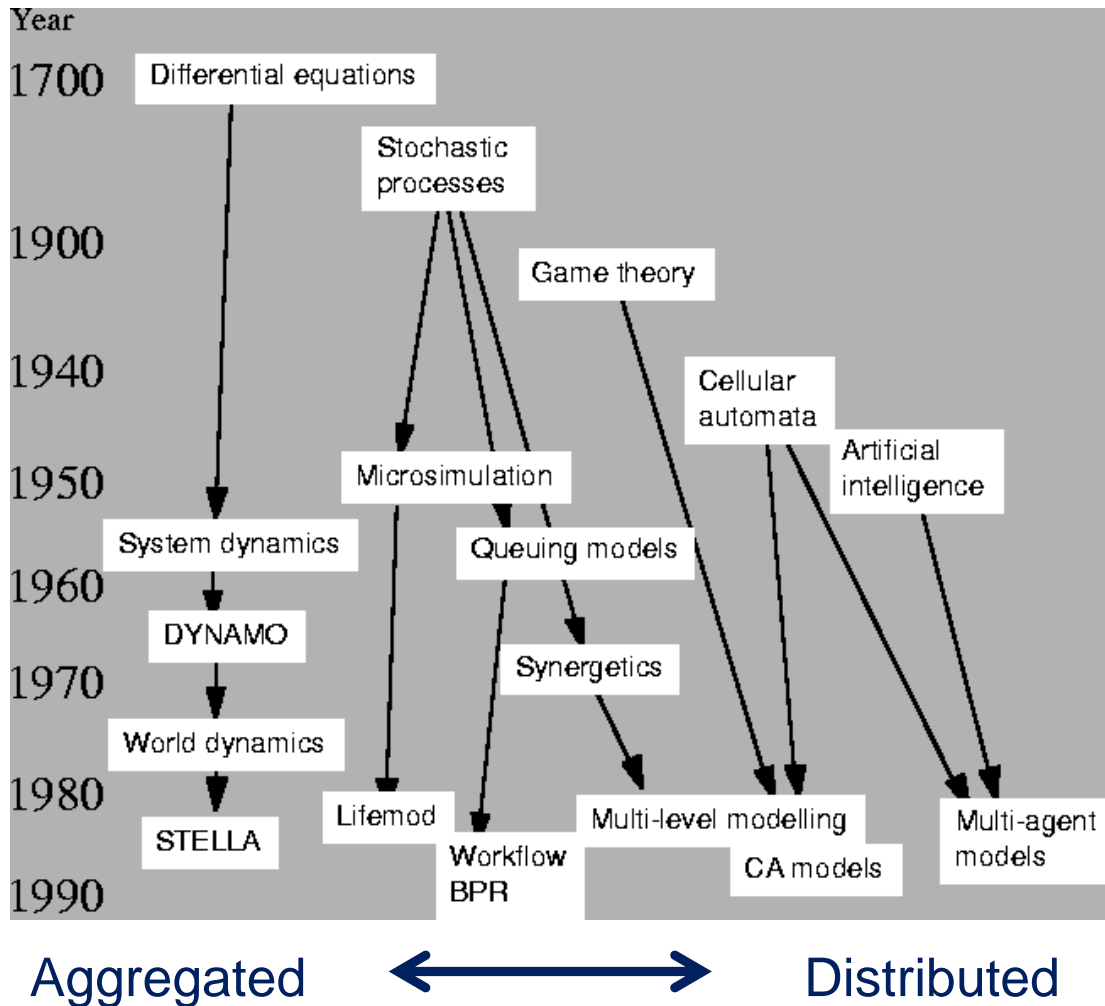


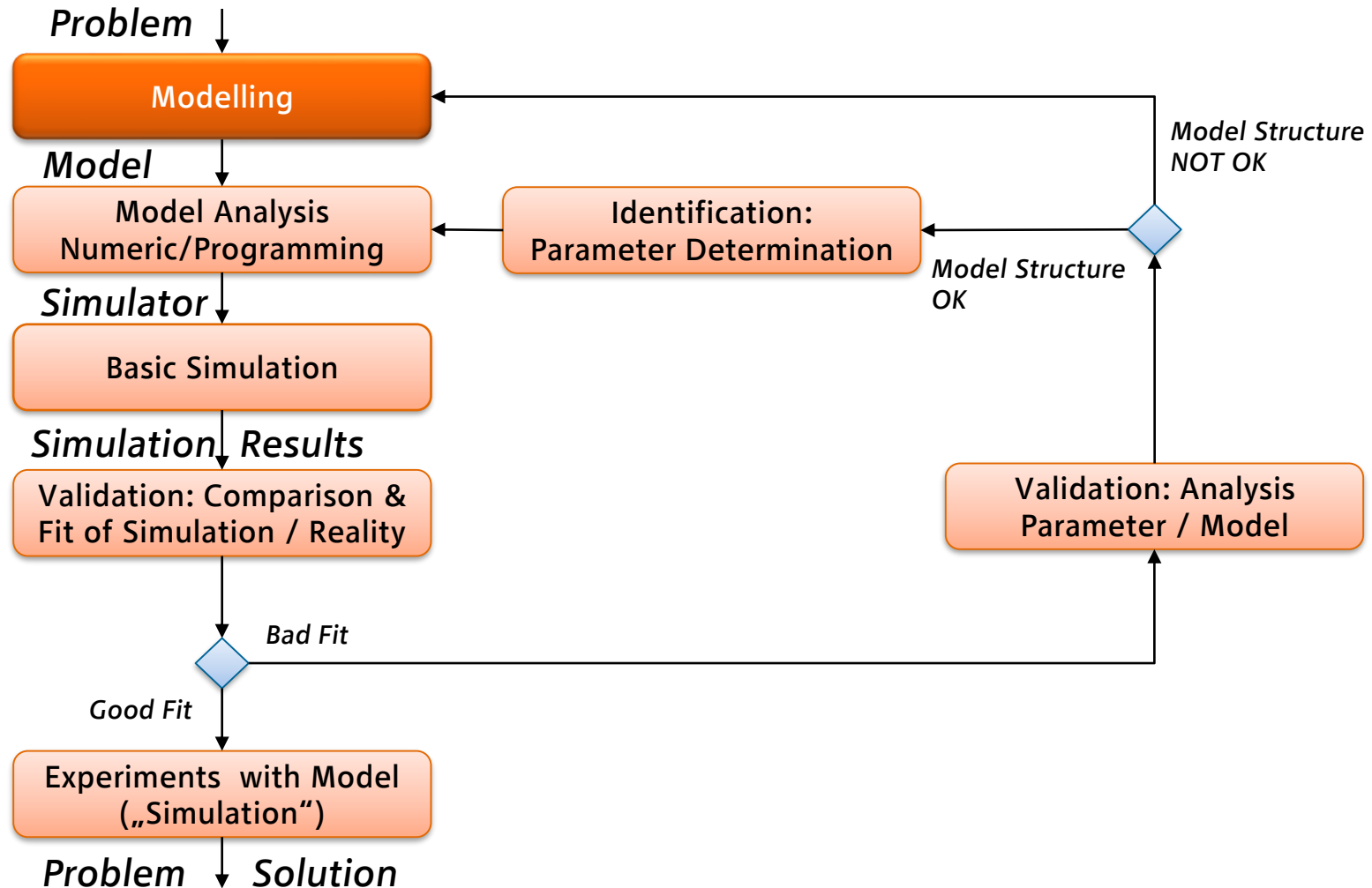
Approaches for Soft Sciences Simulation

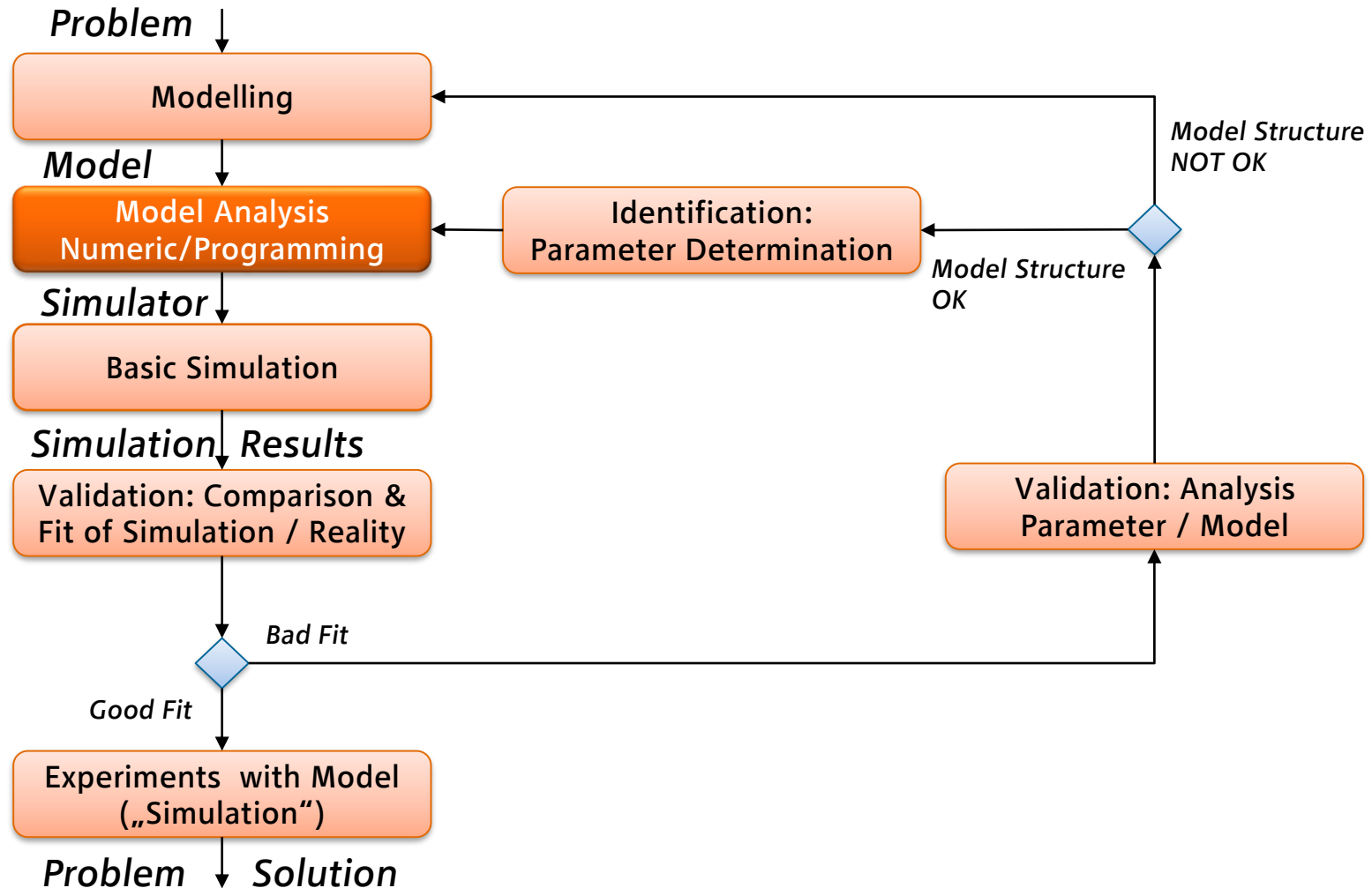


(Troitzsch)

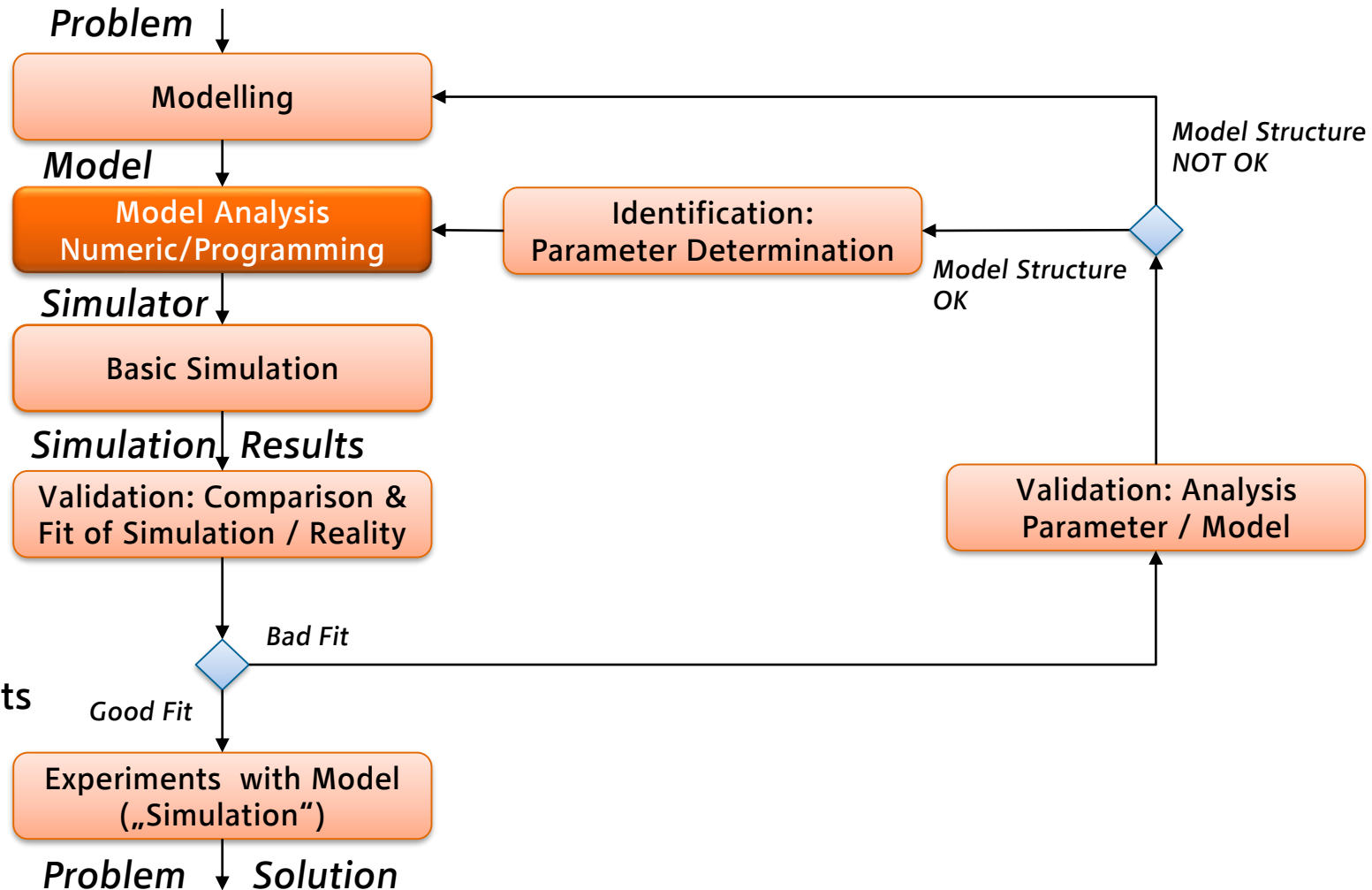
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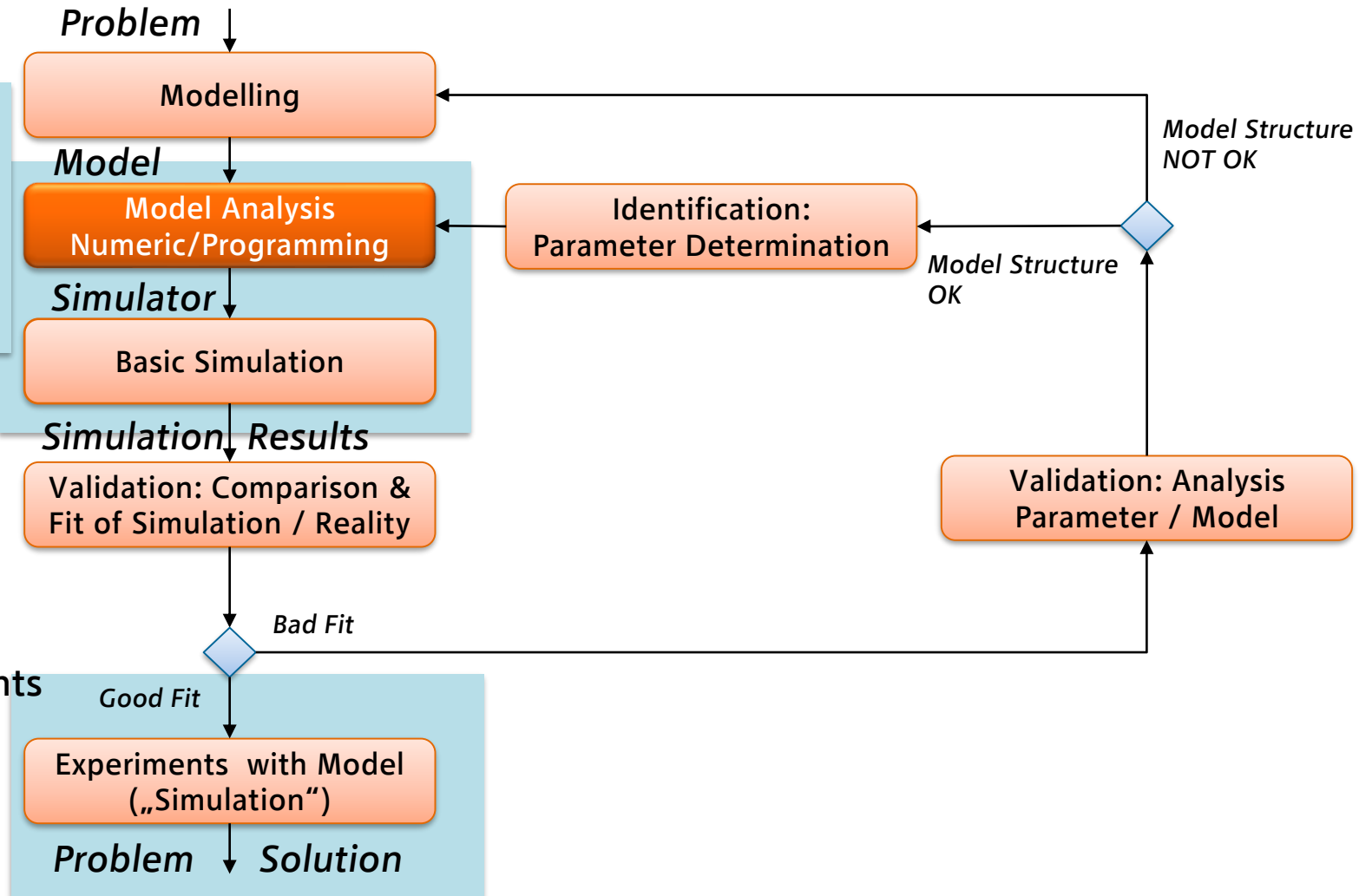




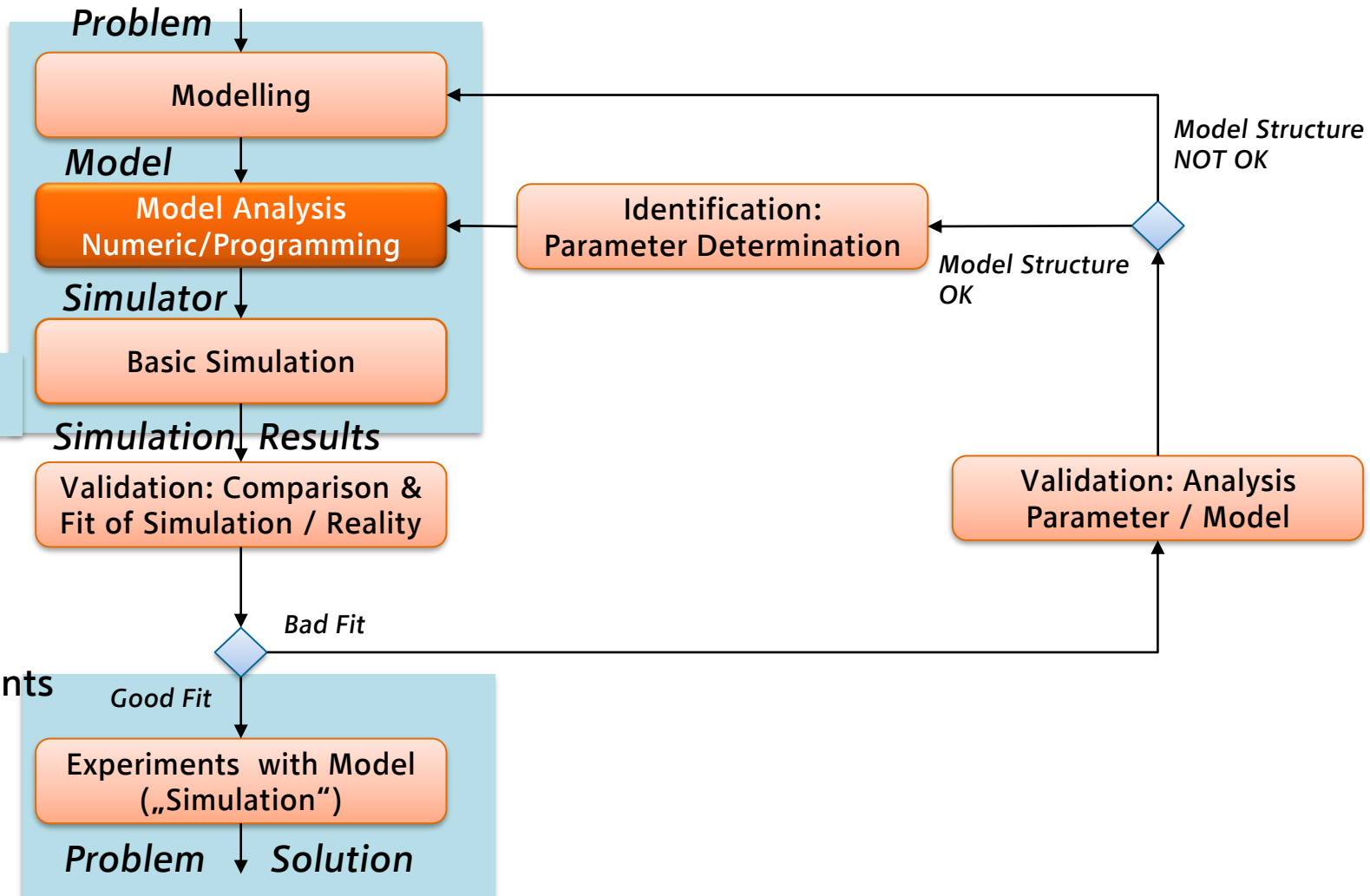
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- simulation languages
- Simulators
- Simulation systems
- Simulation Environments



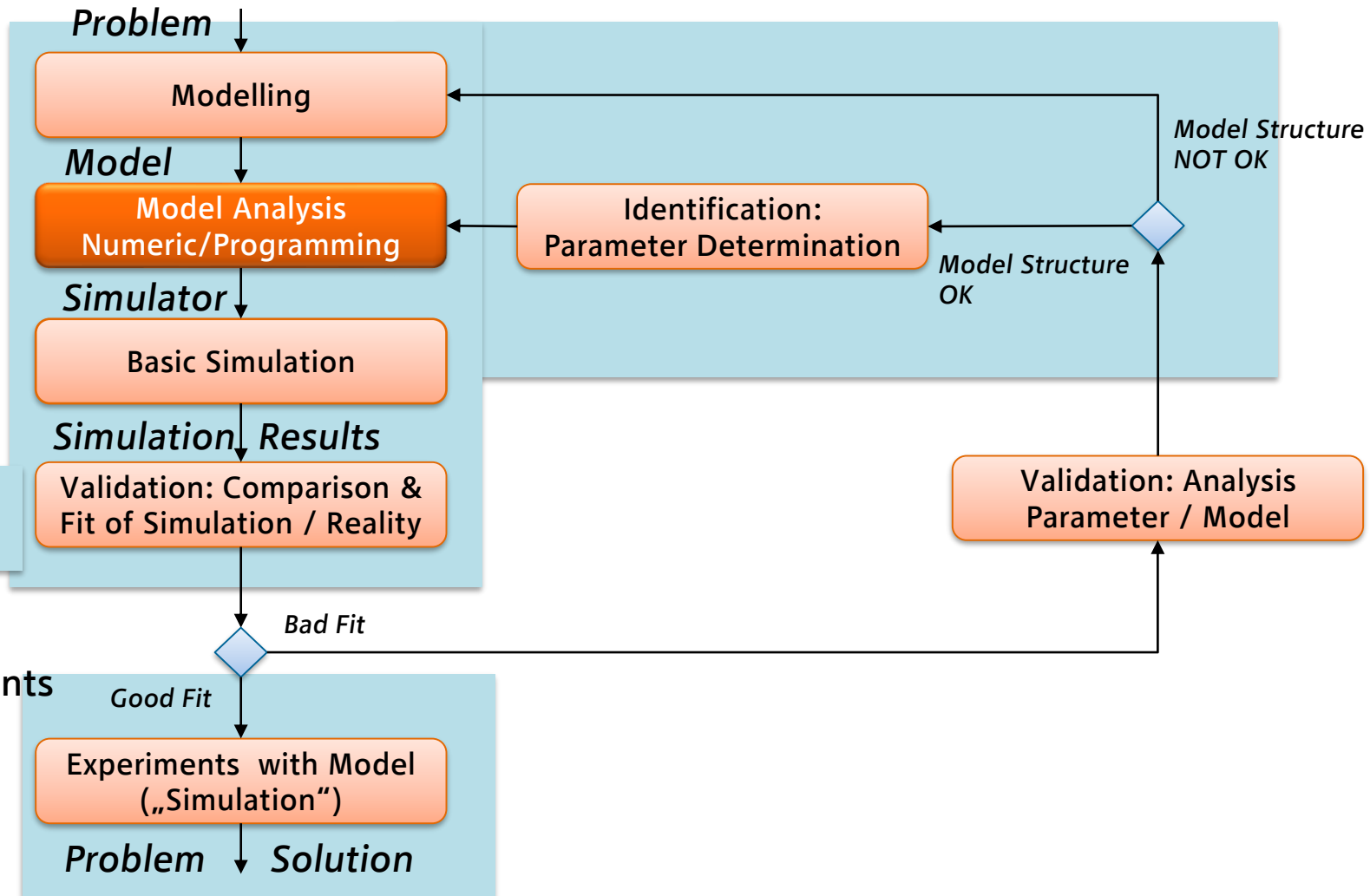
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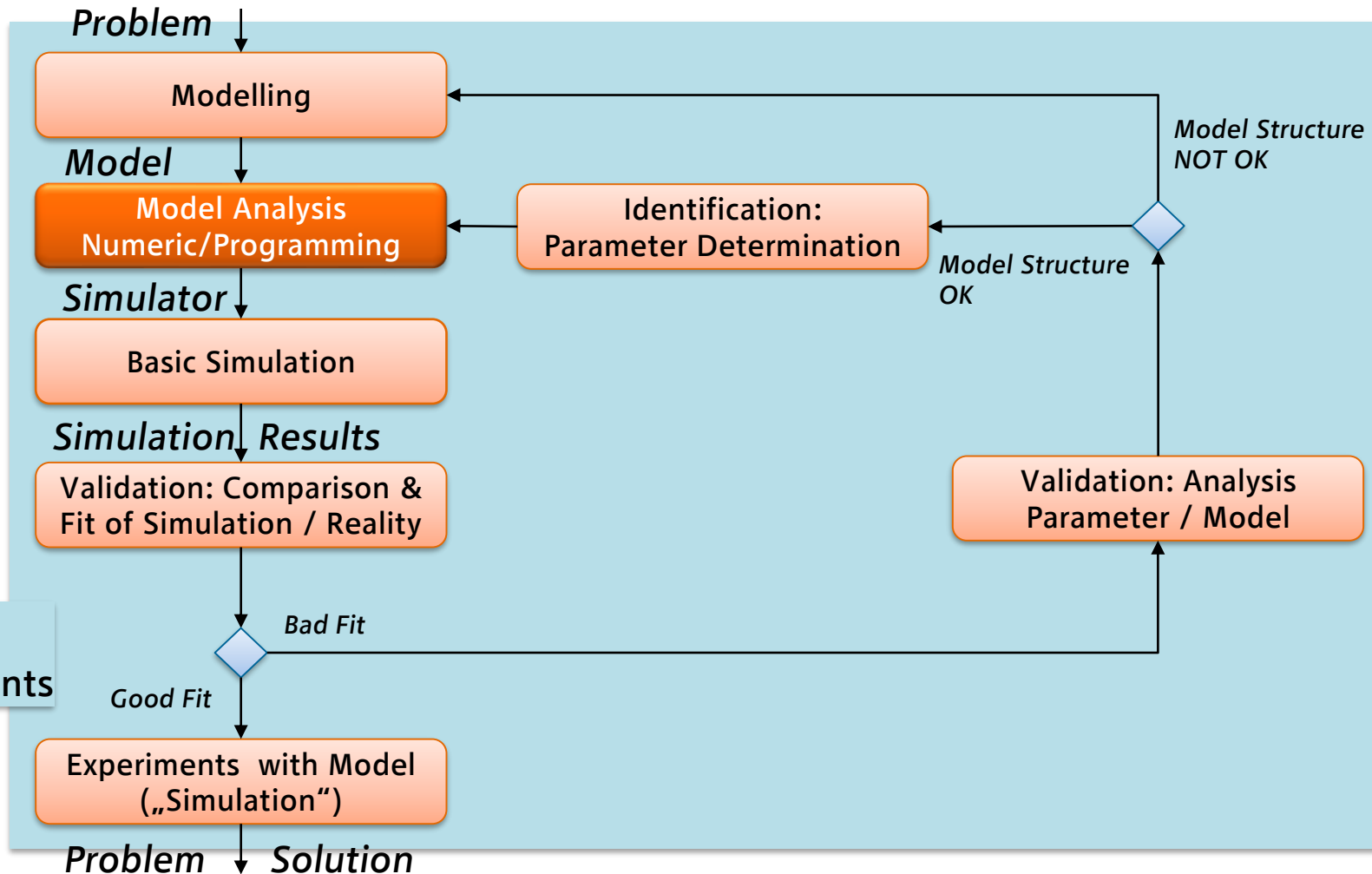
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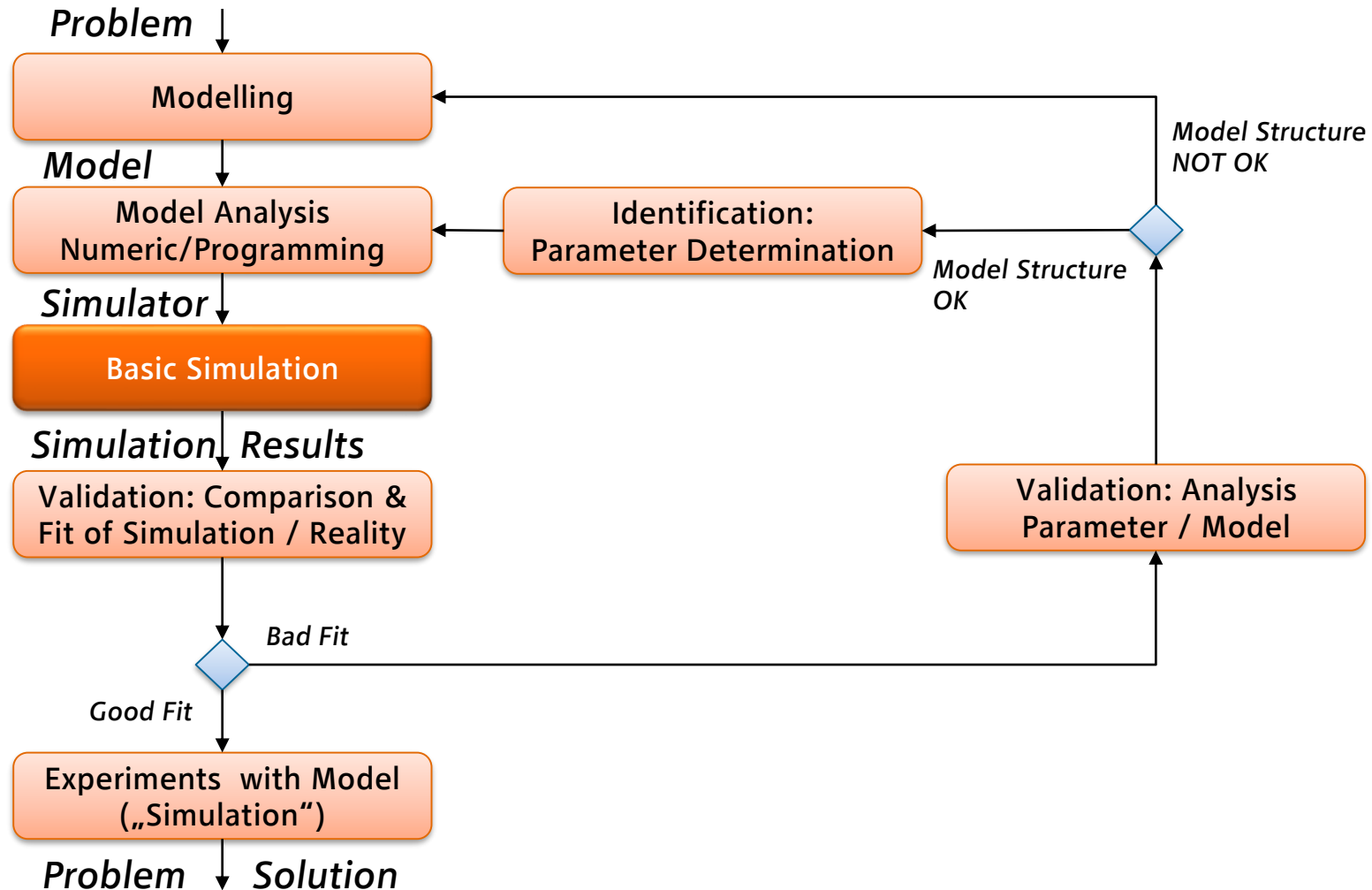


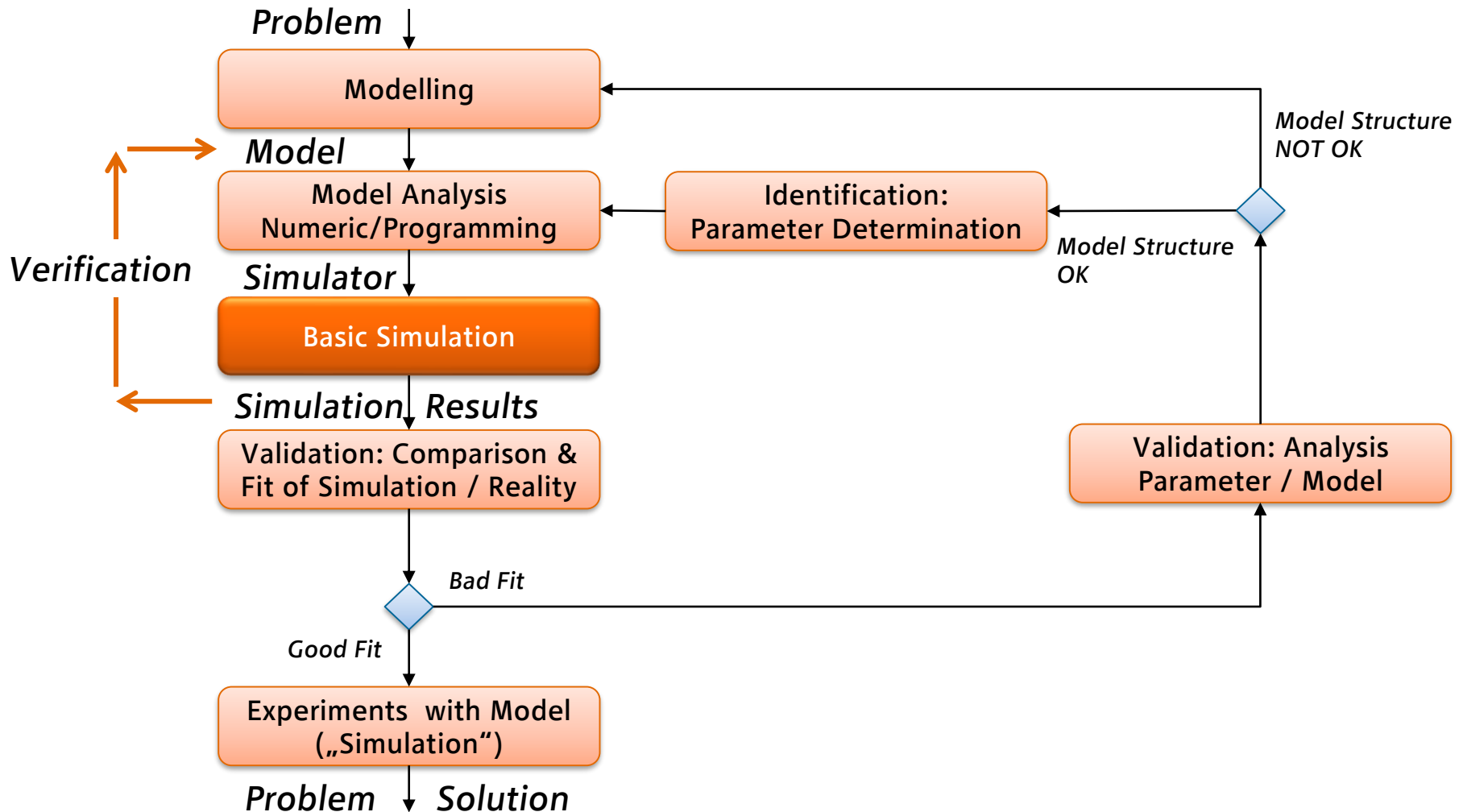
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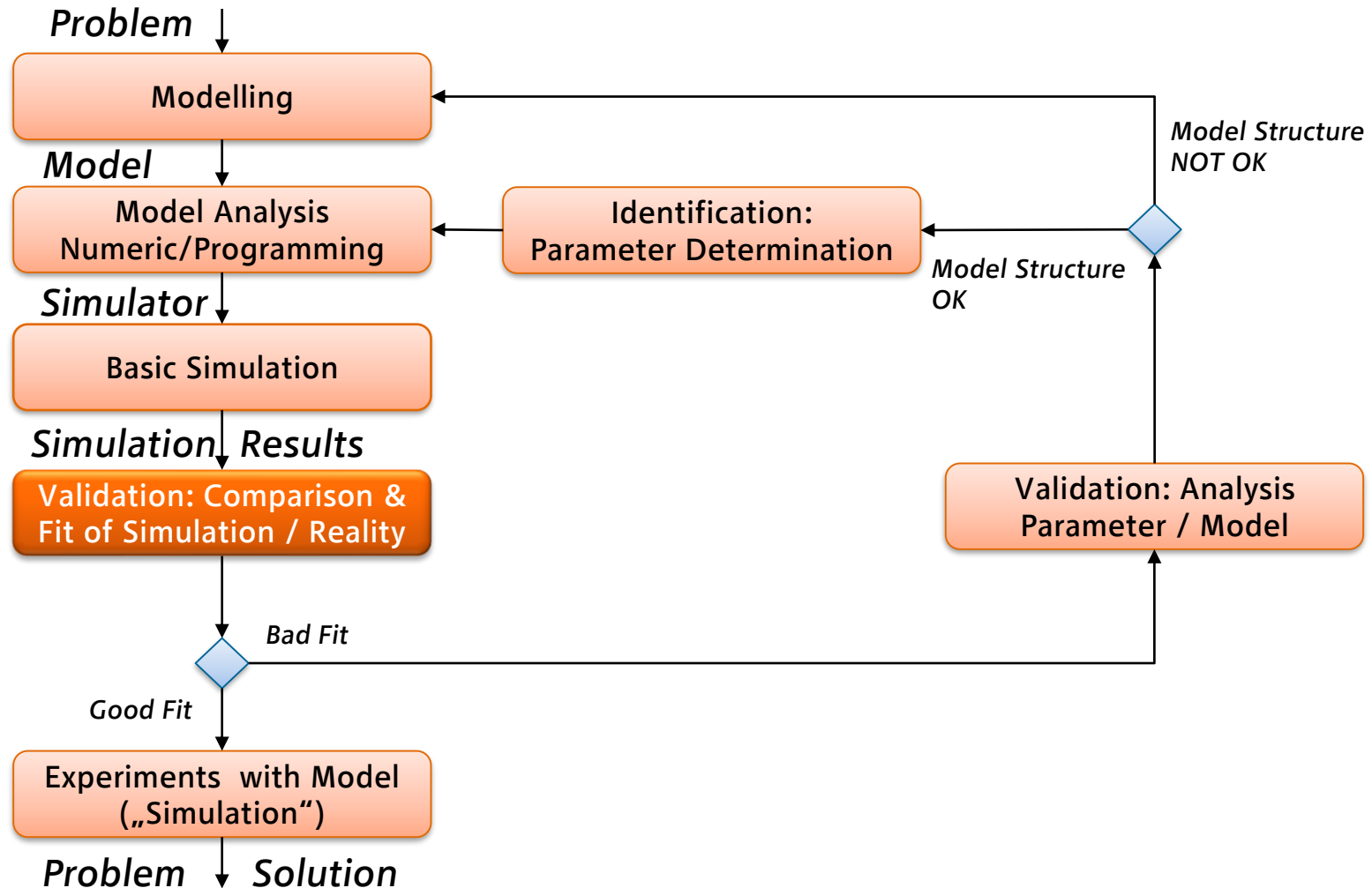


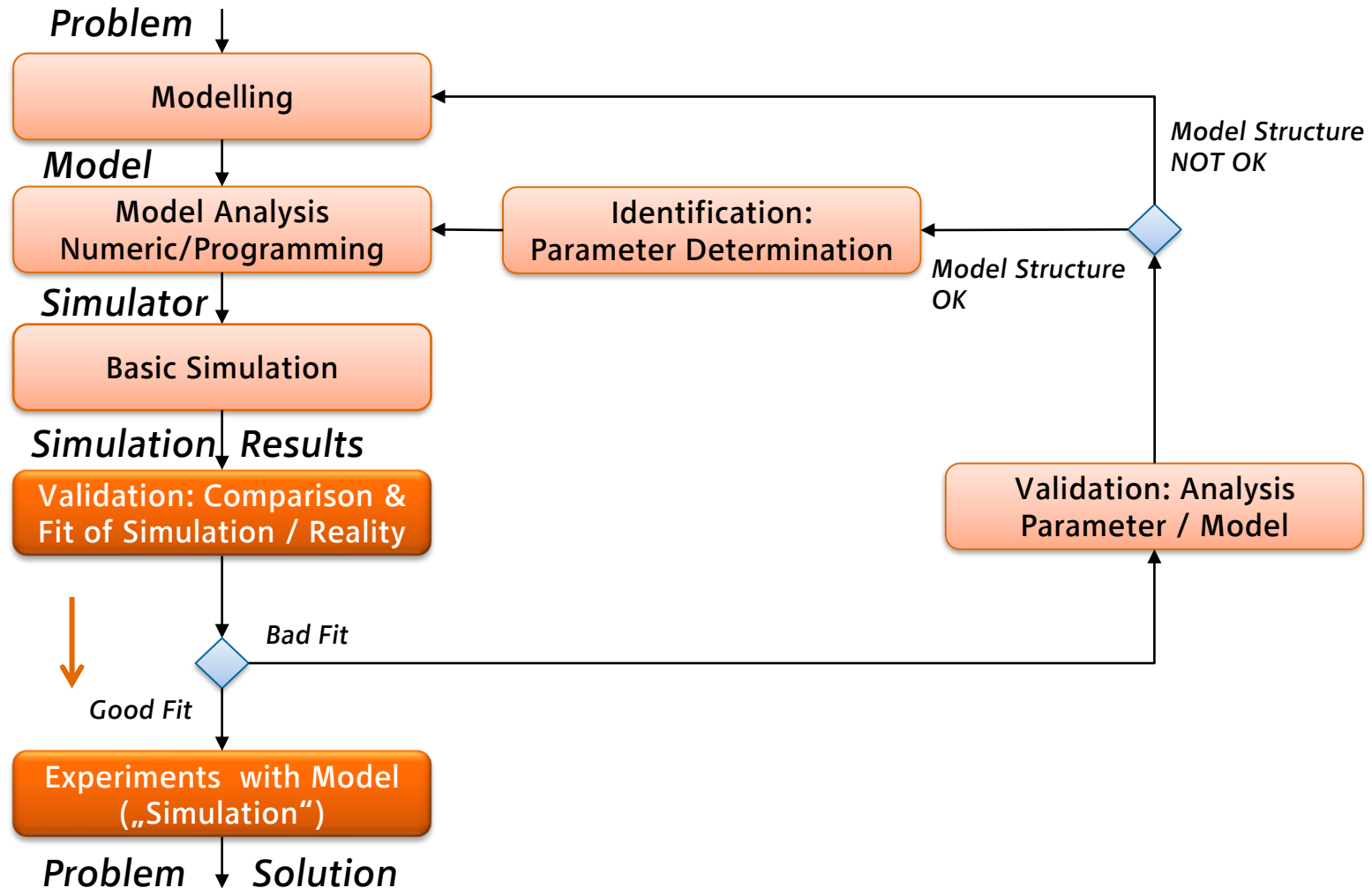
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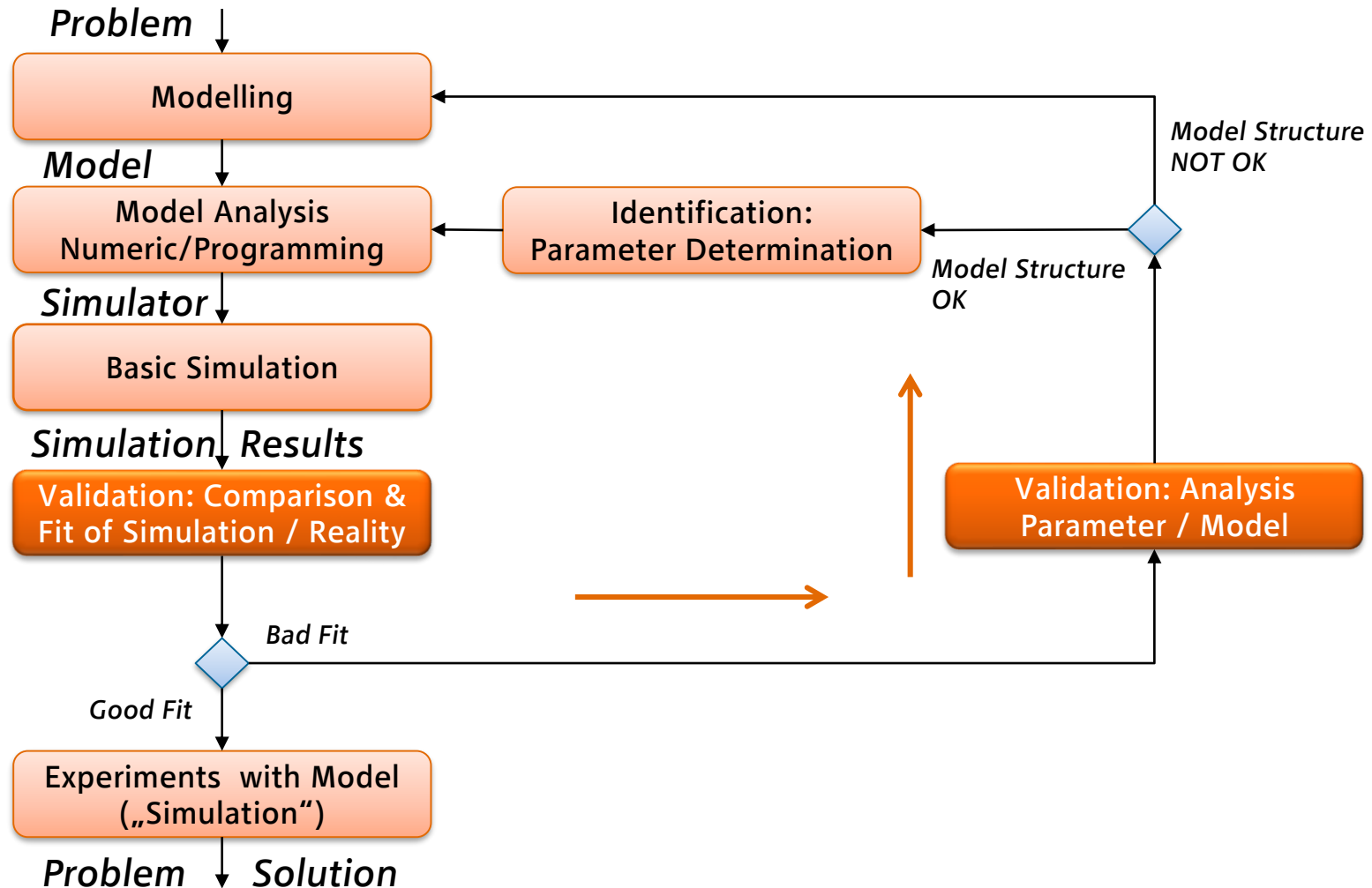


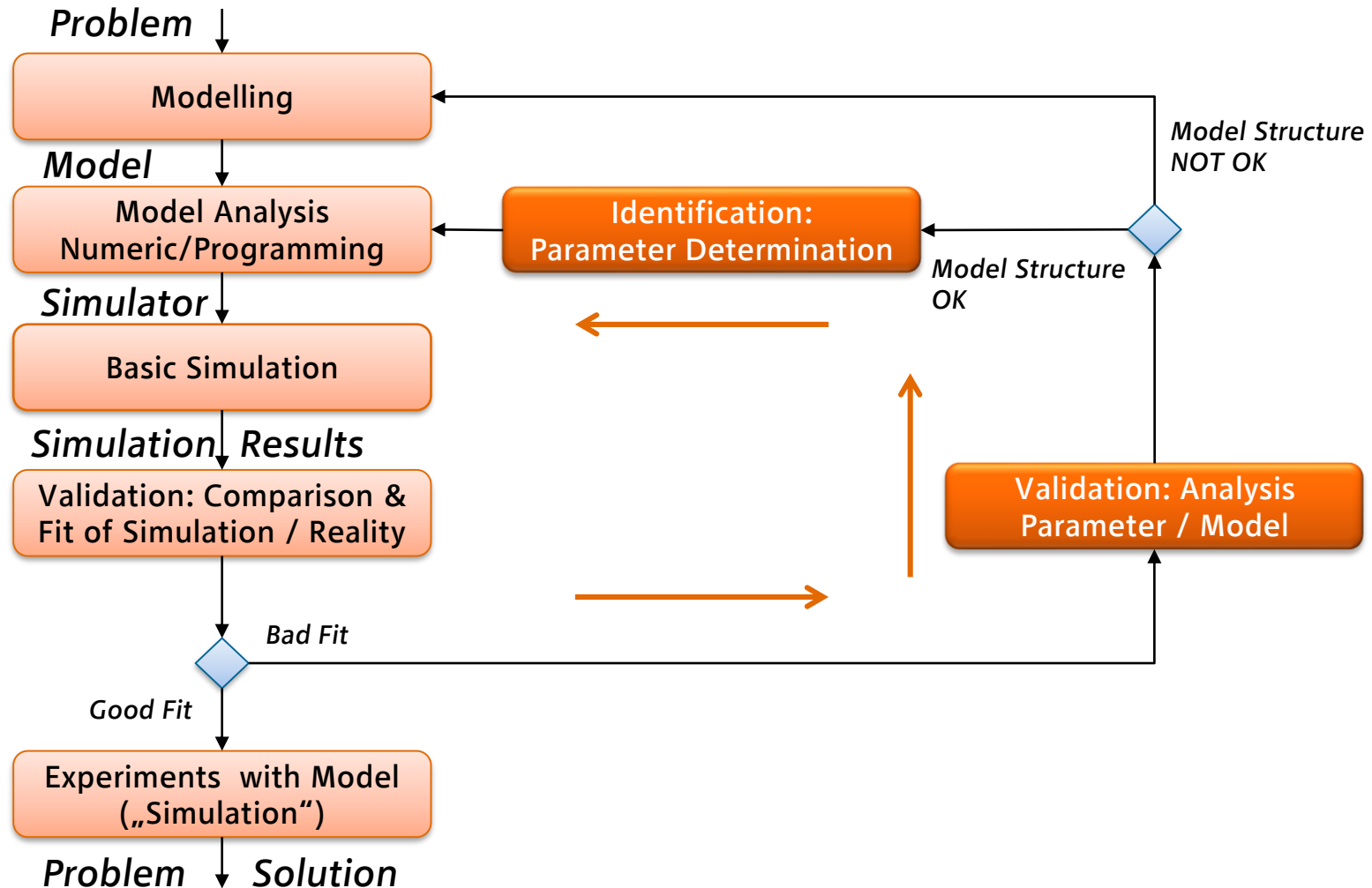






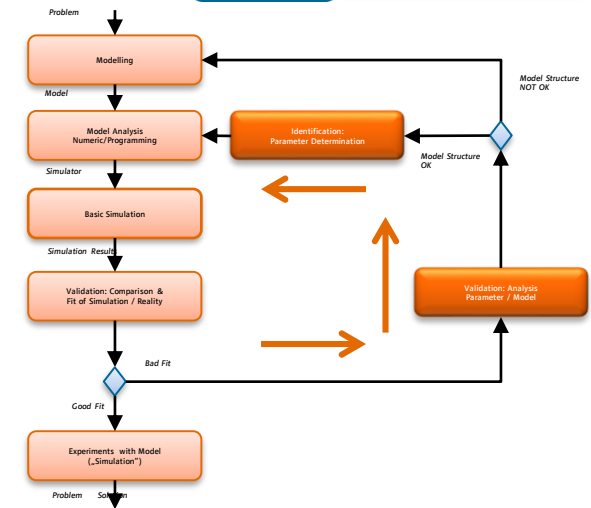
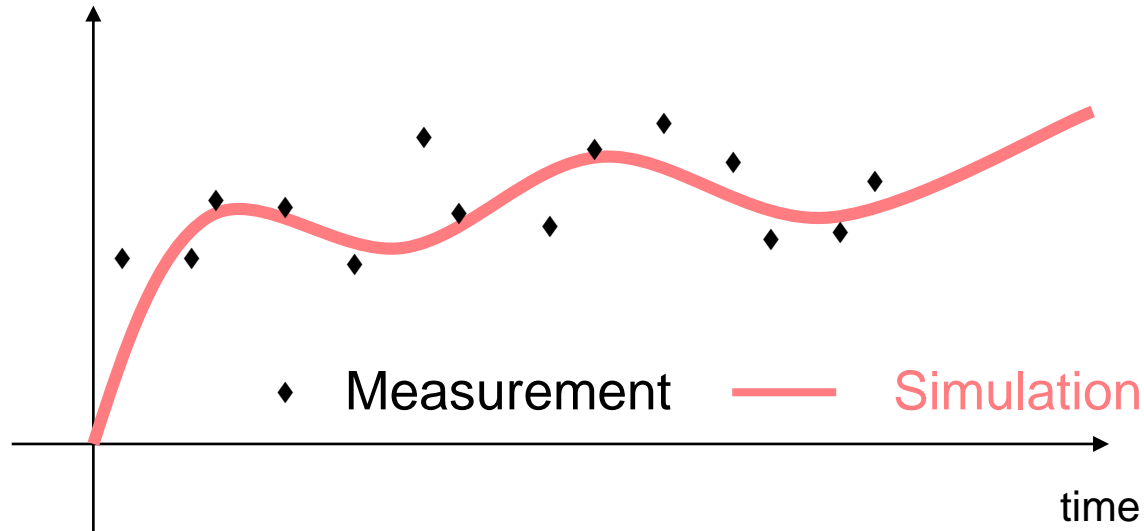


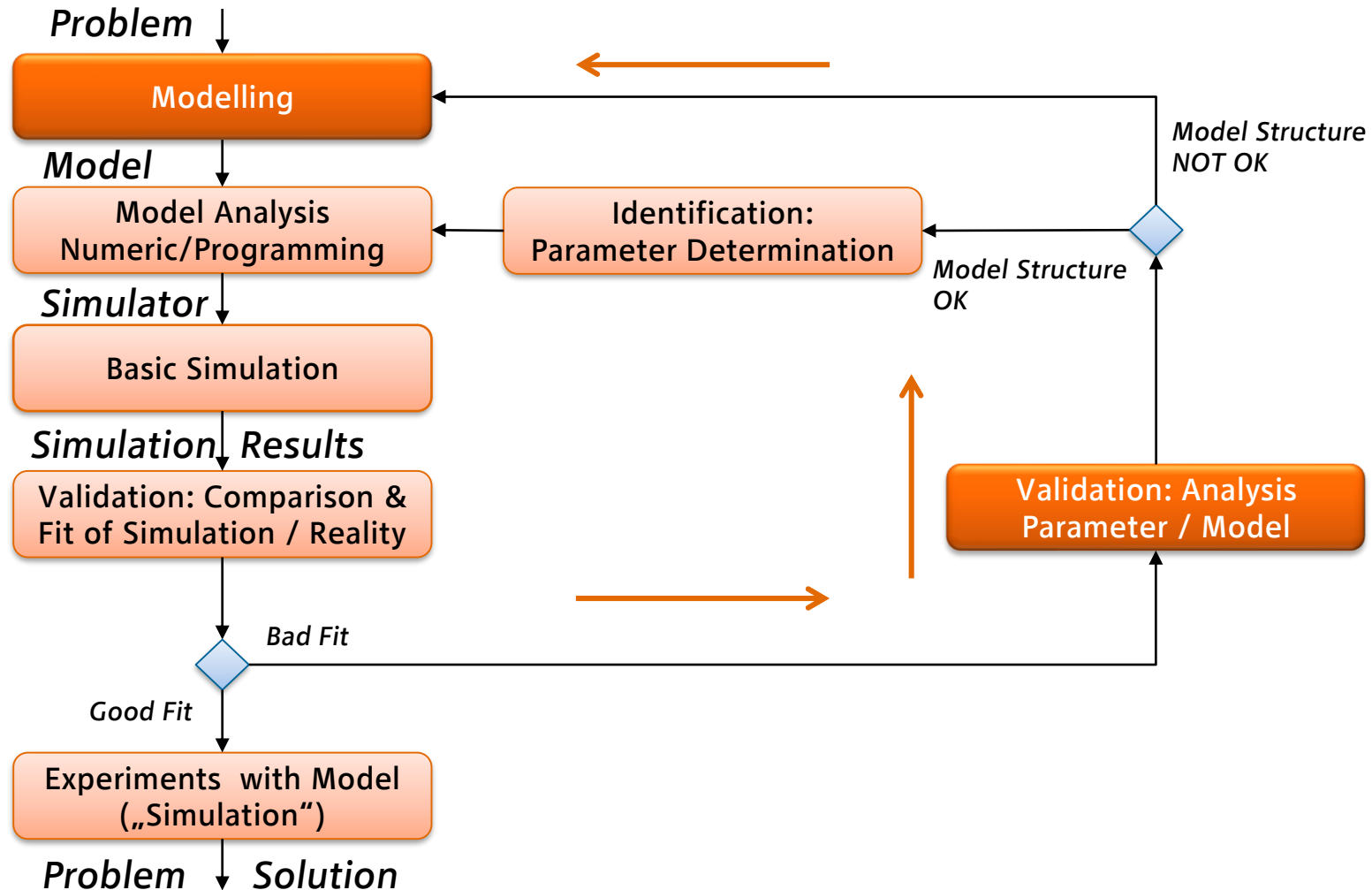


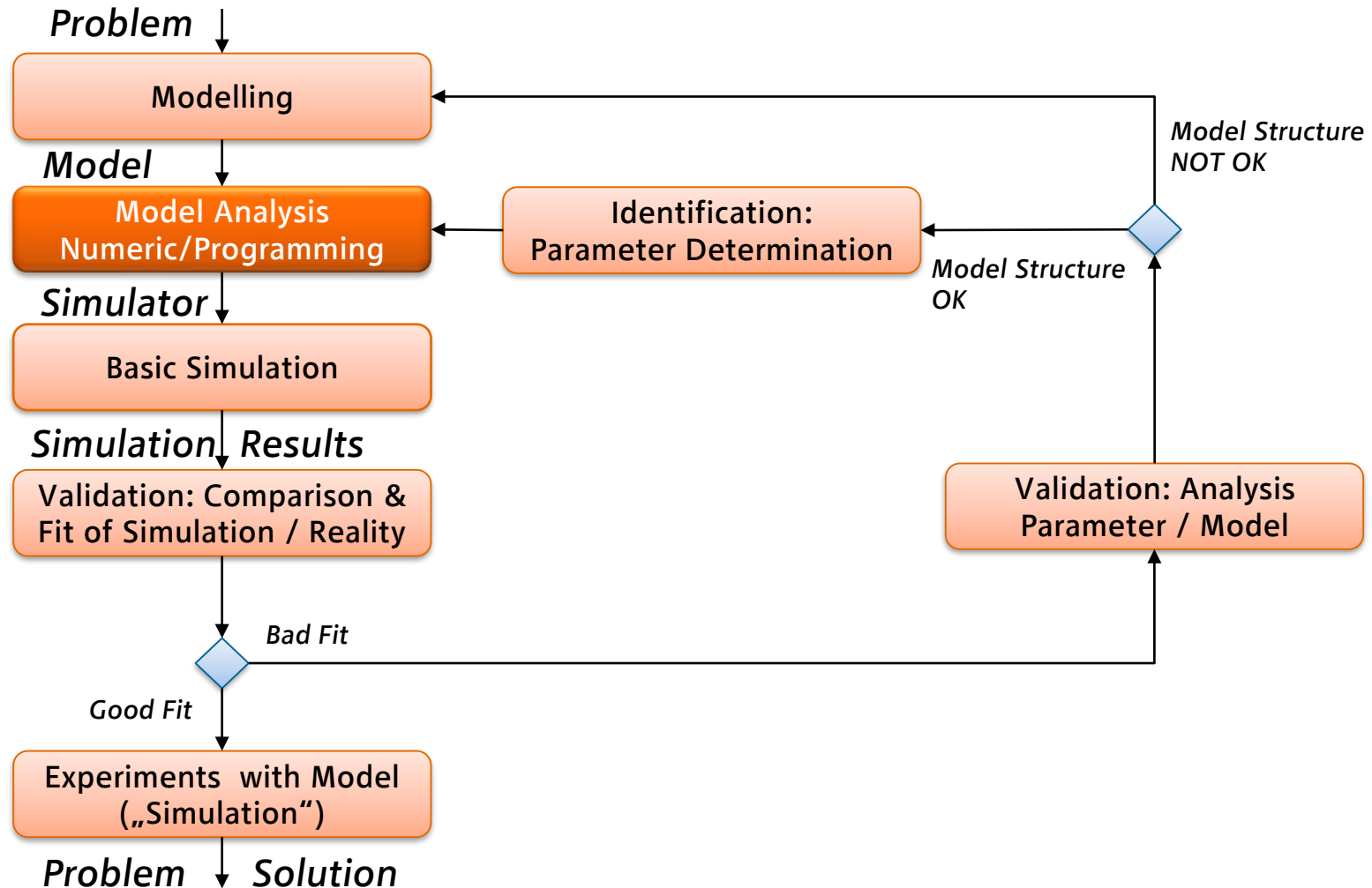


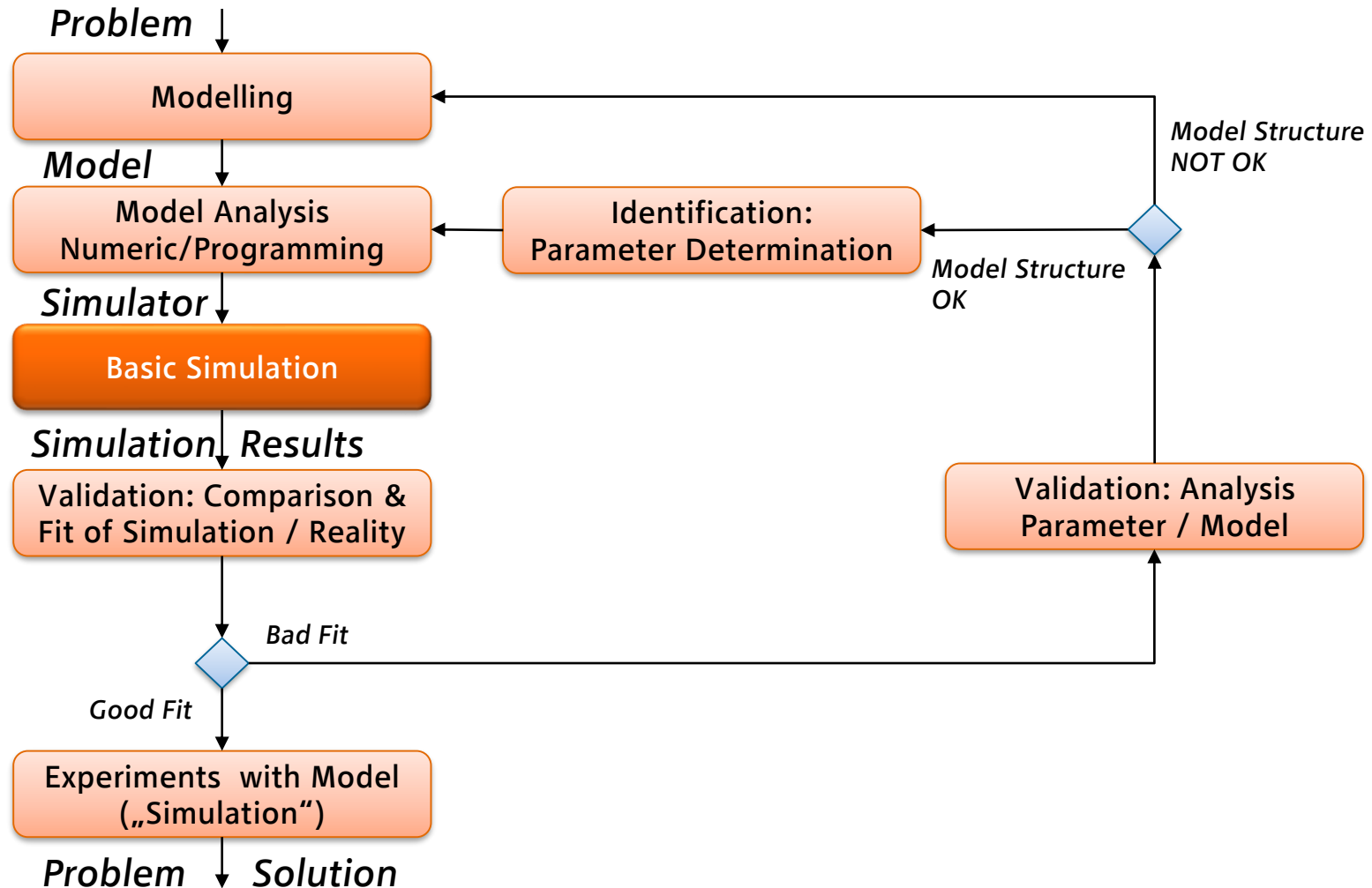
Simulation Circle

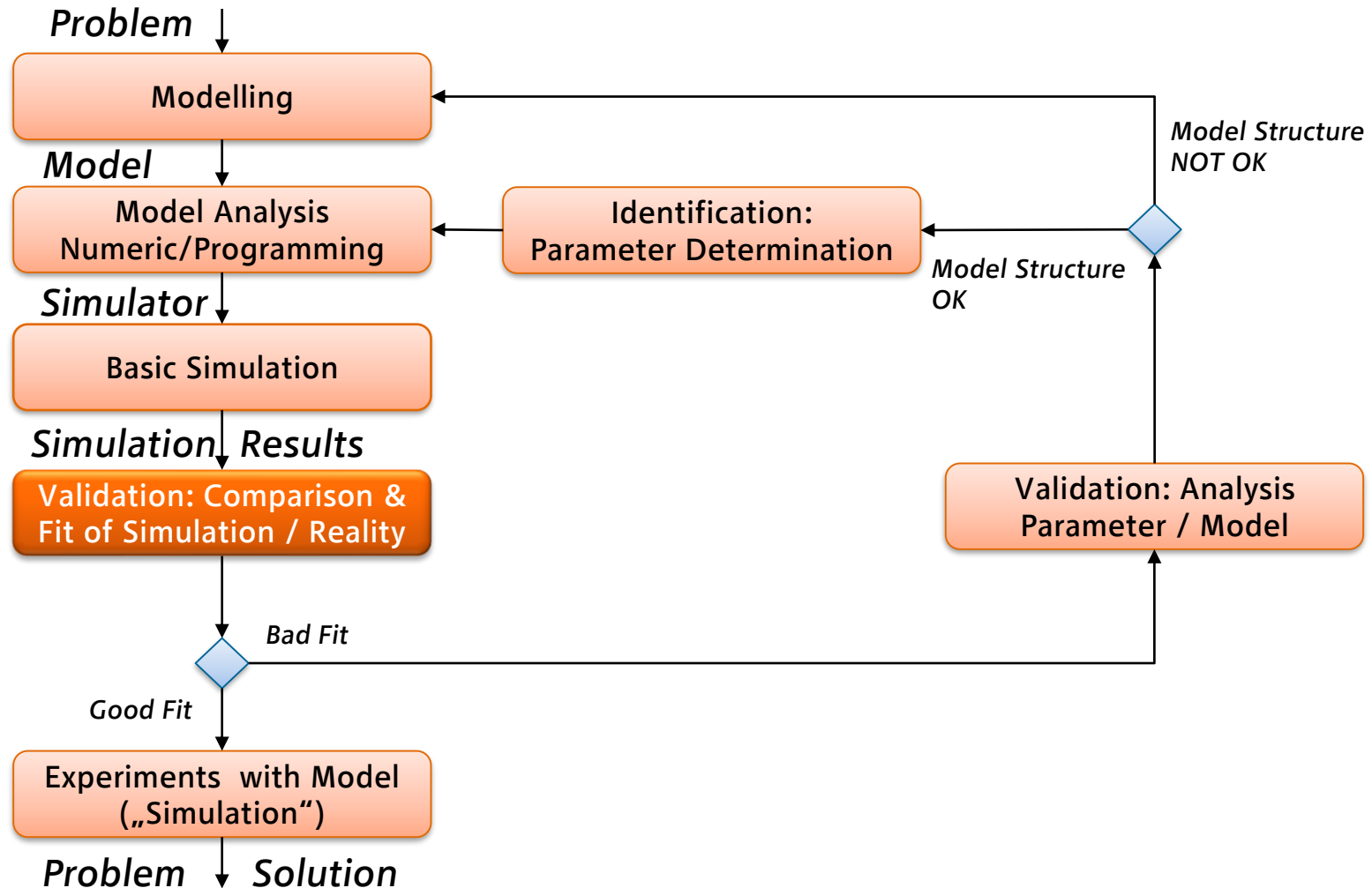
State,
Observation

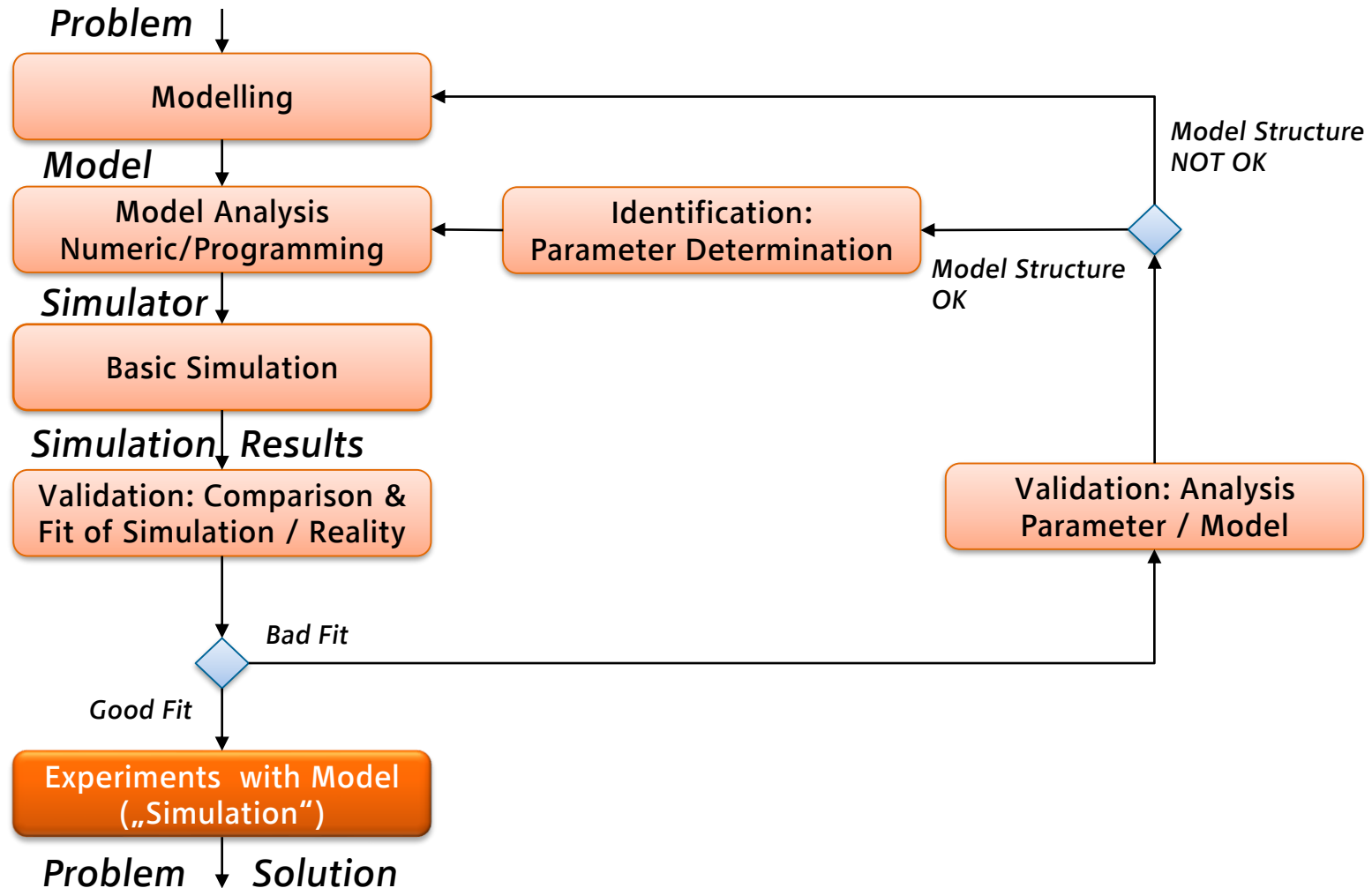


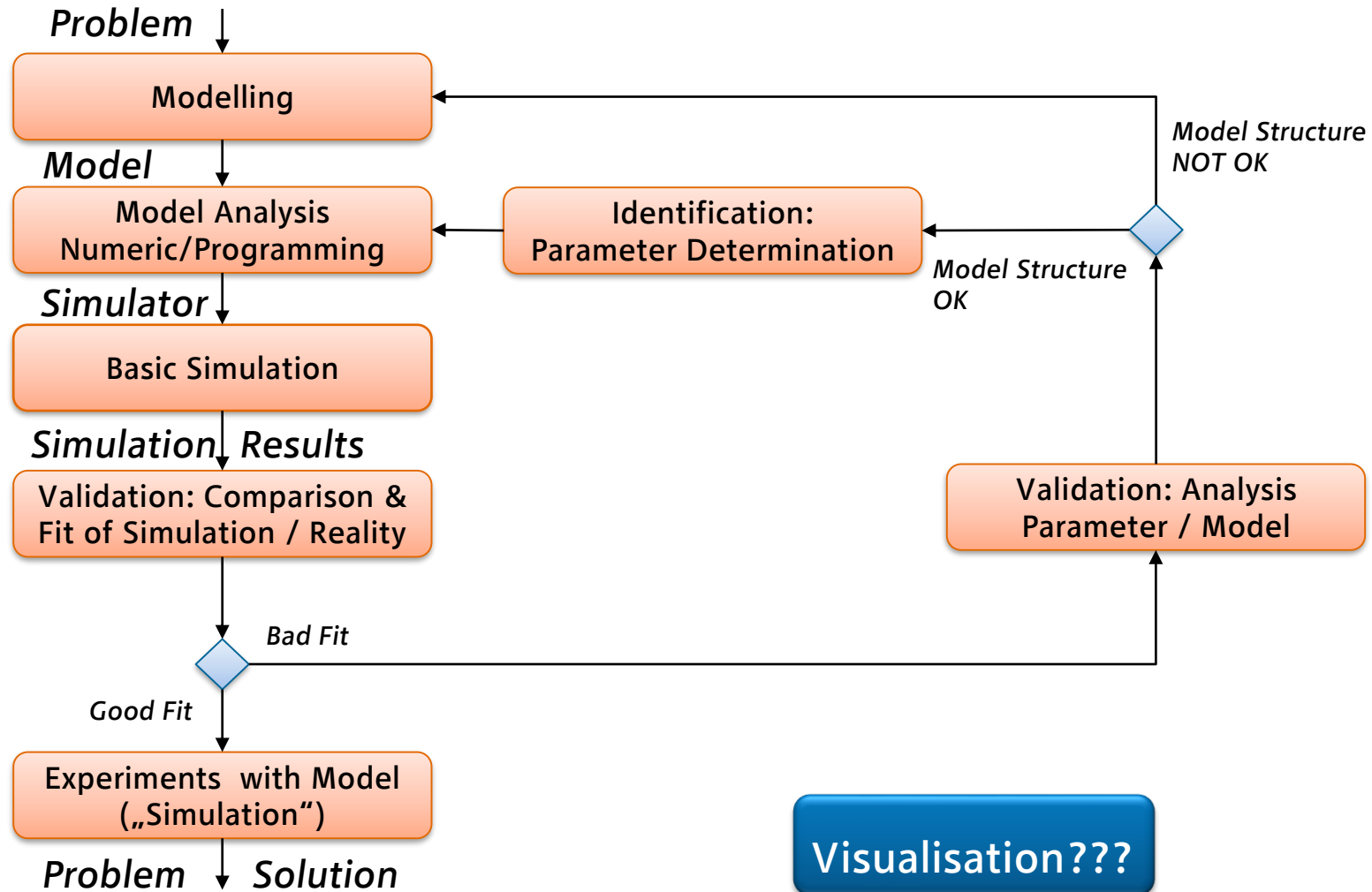


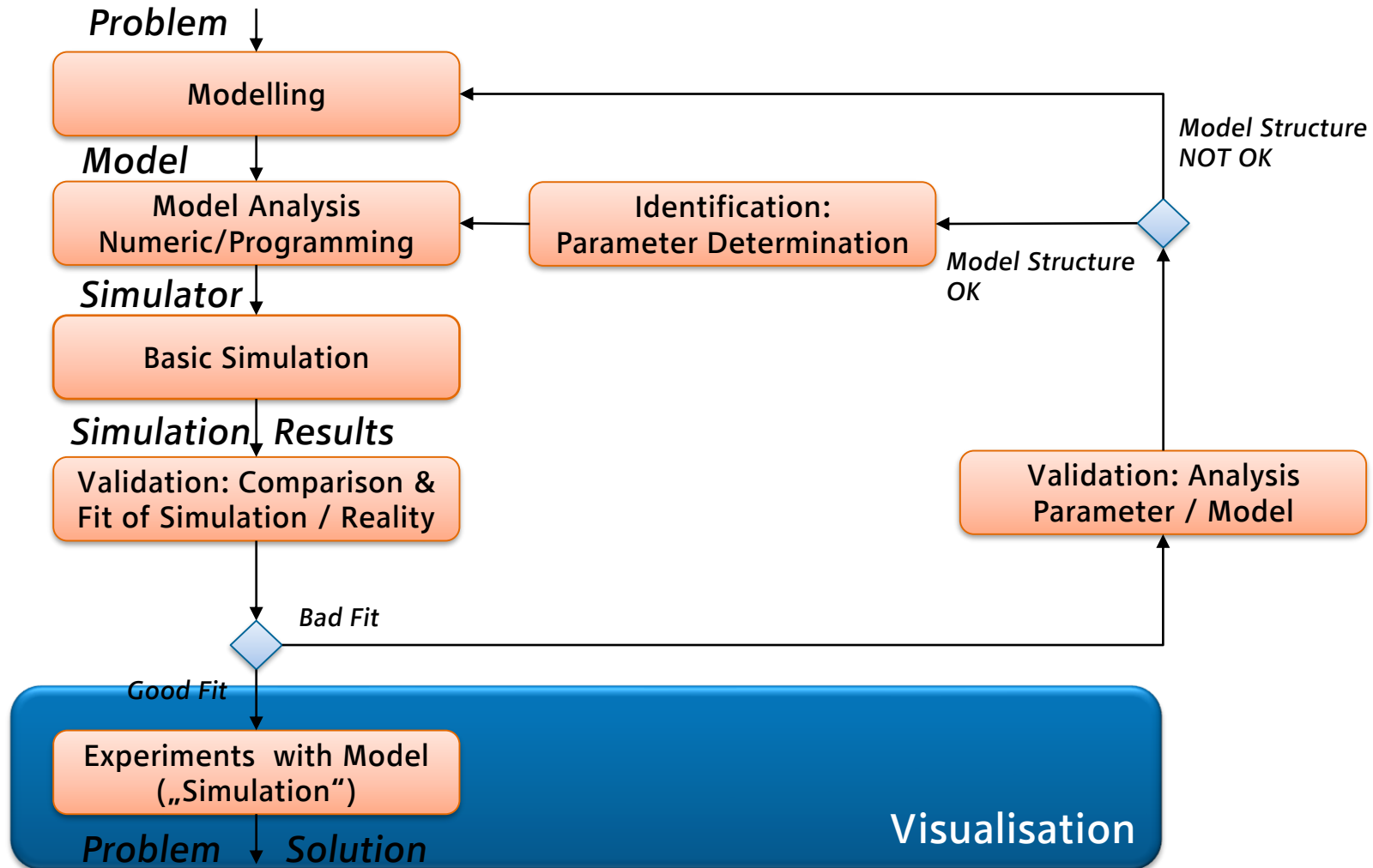


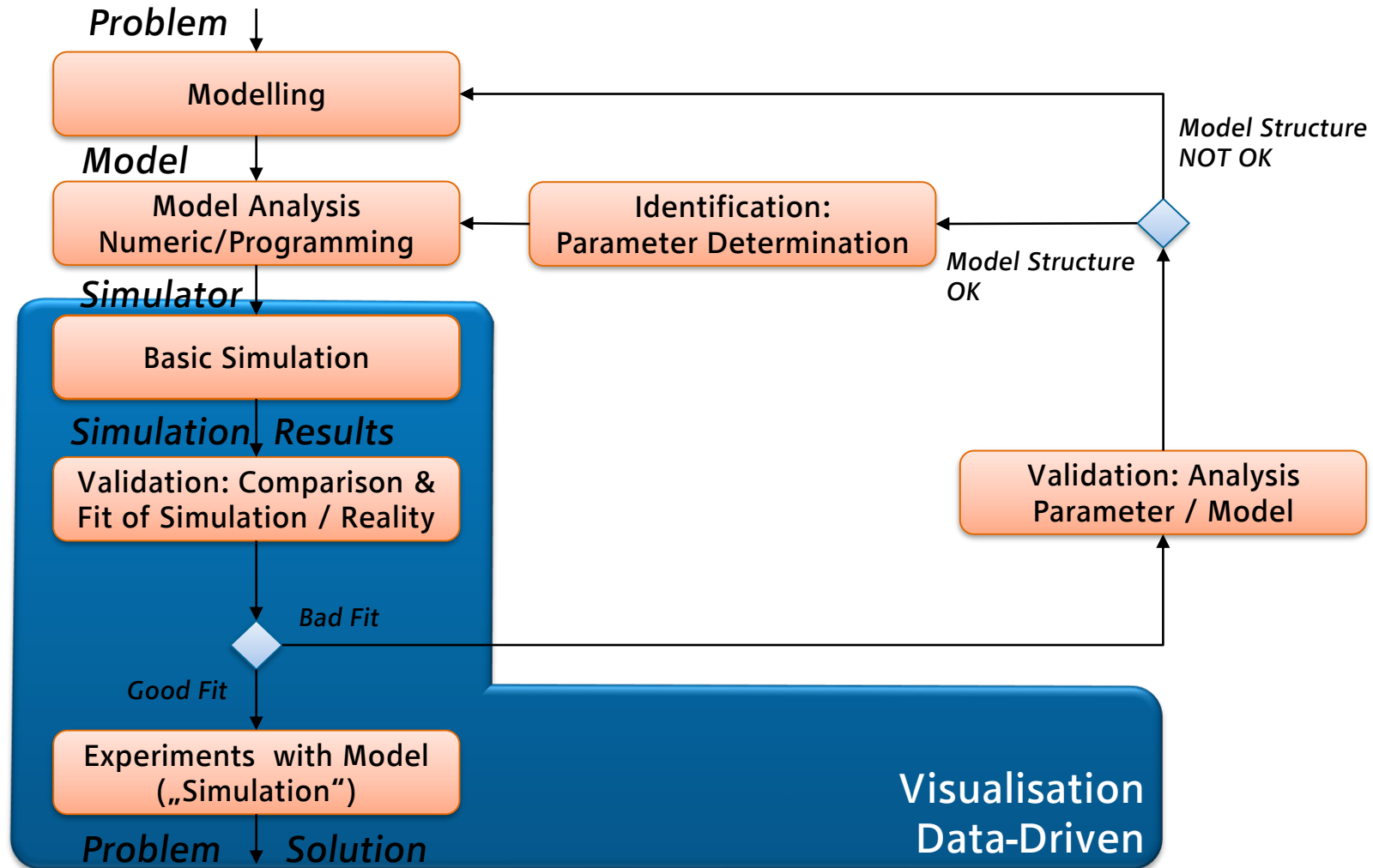


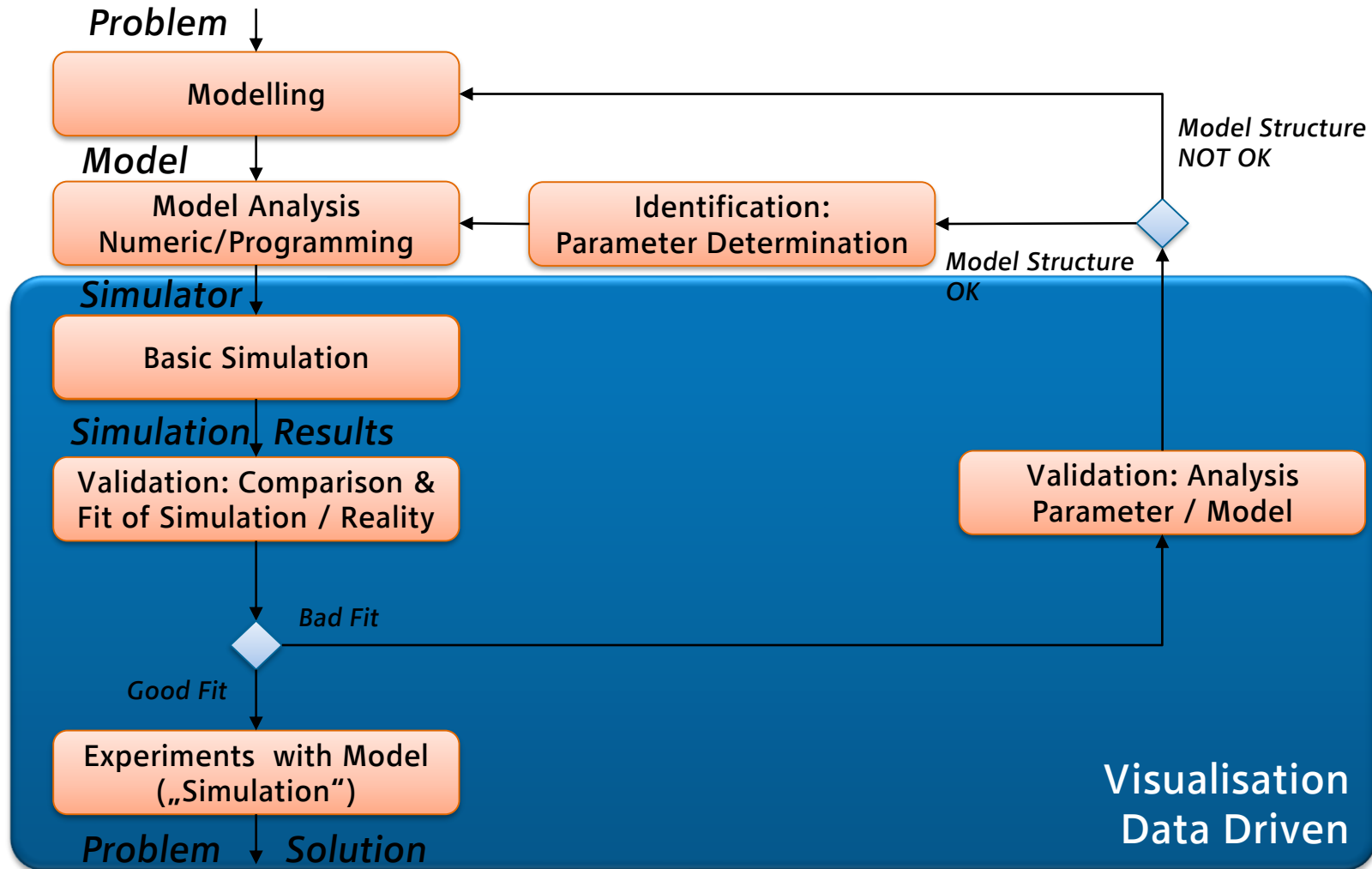


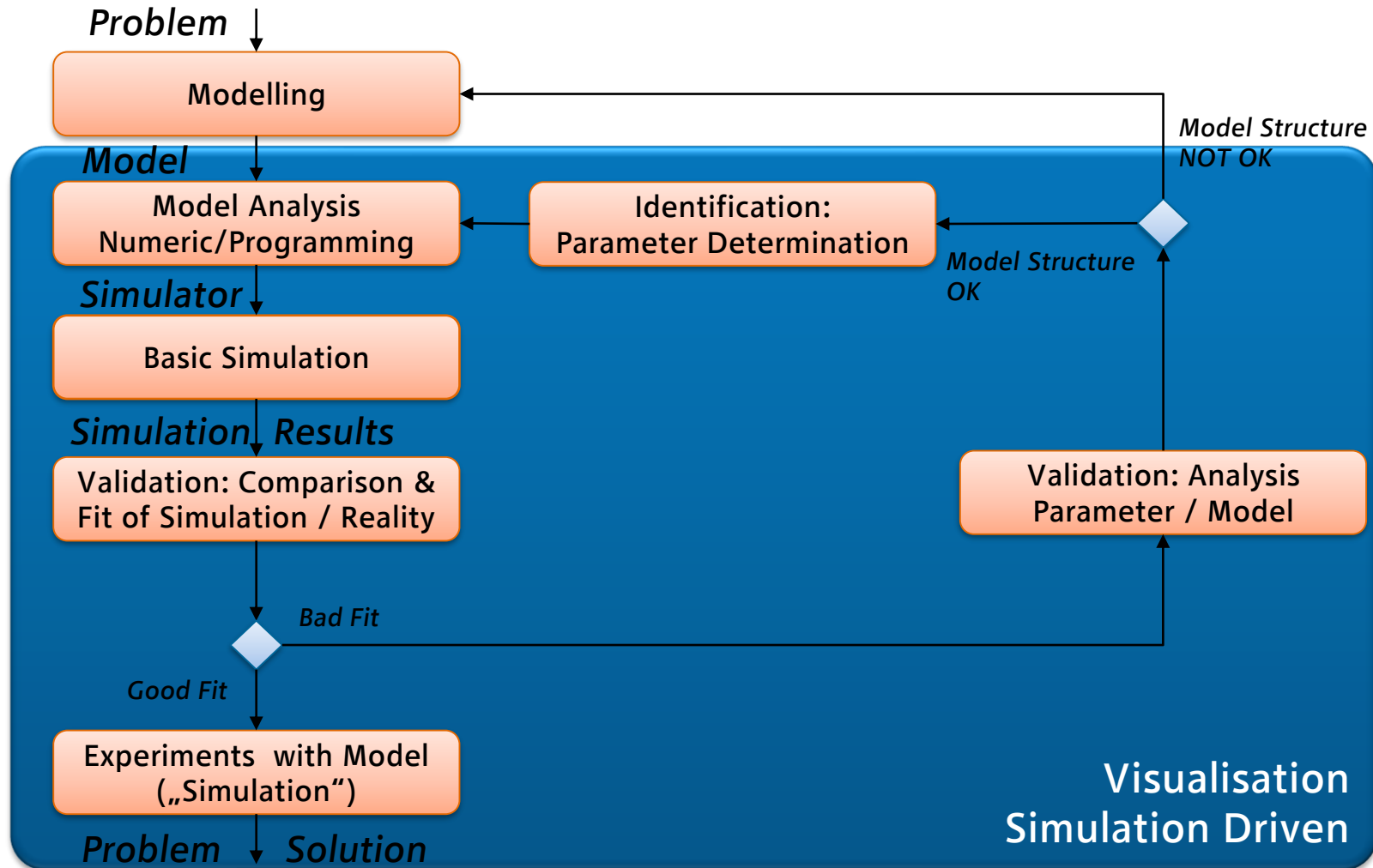


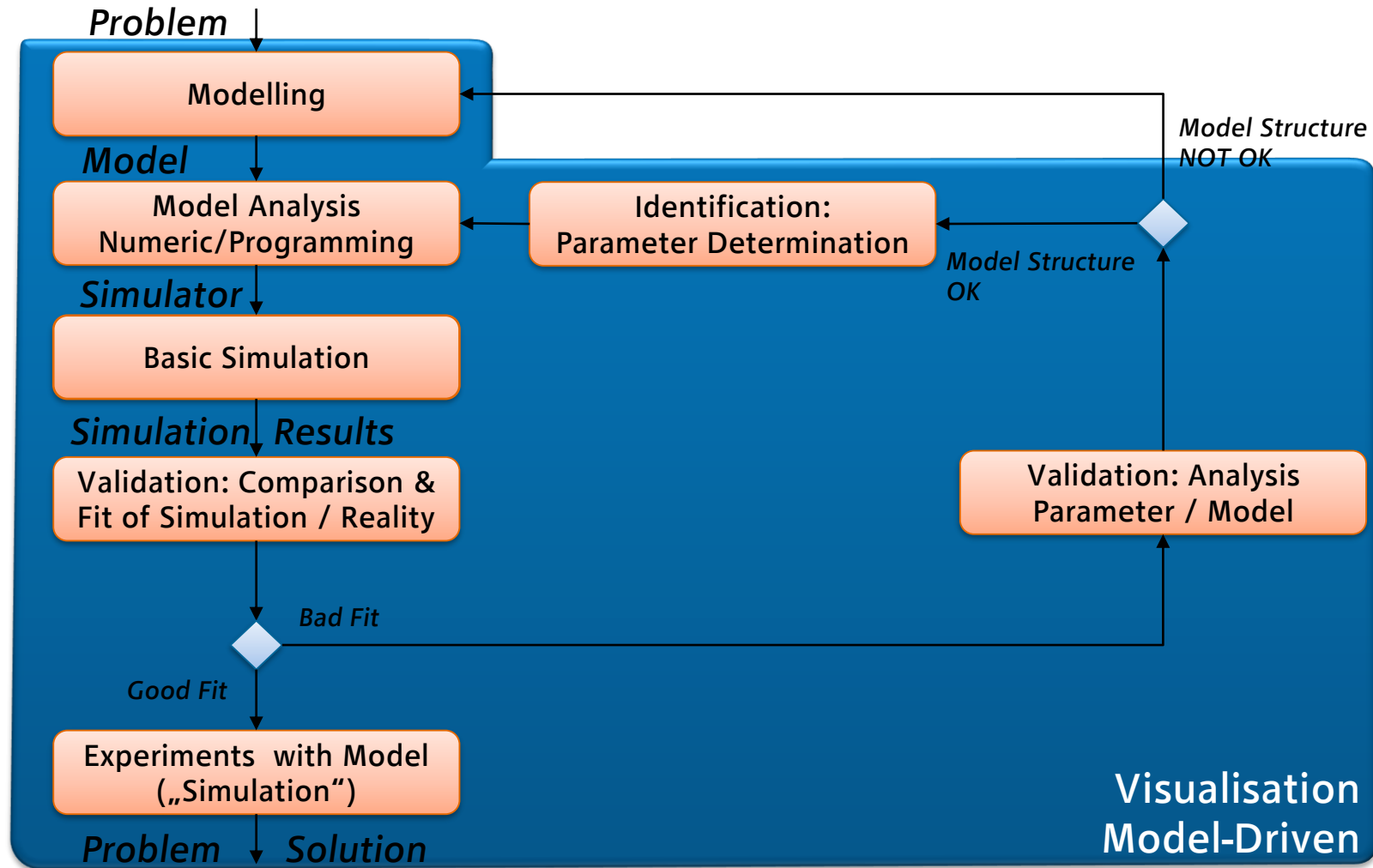






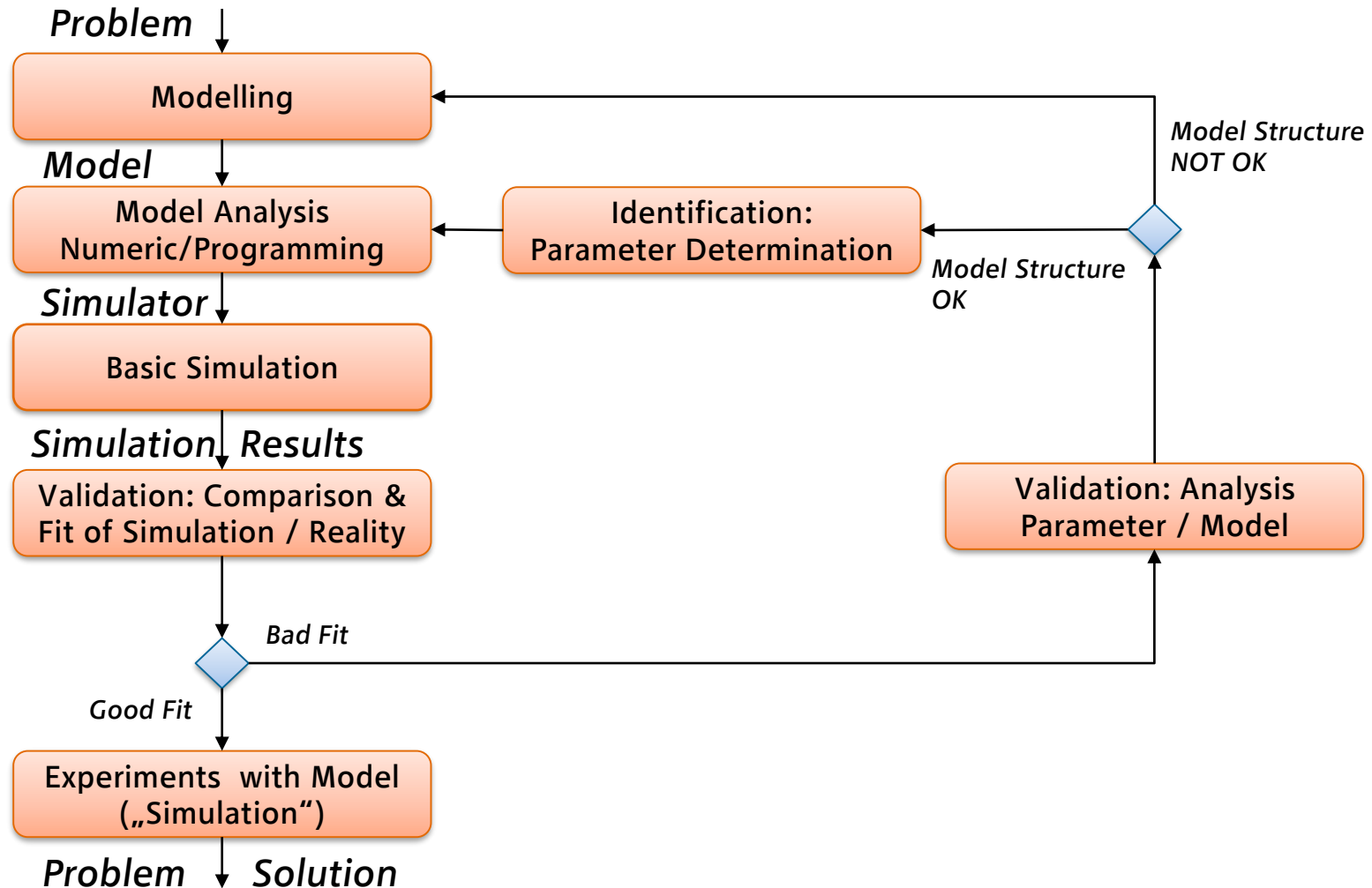






Testcase: Predator-Prey

SIMULATION CIRCLE



Forrester, 1961

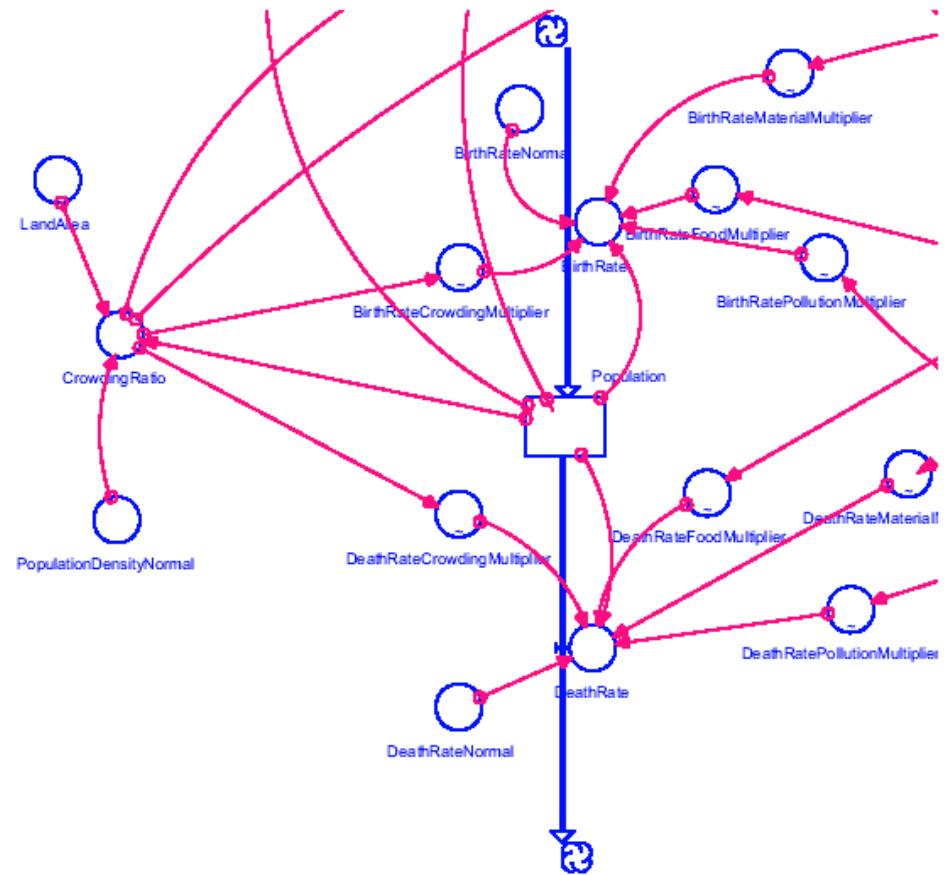
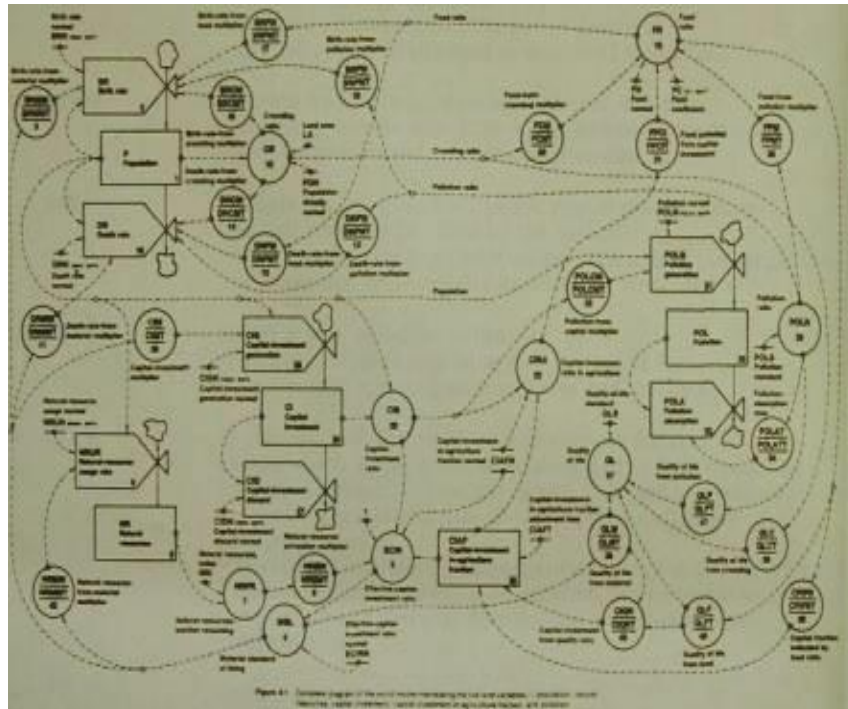
System Dynamics is a field that resulted from the pioneering efforts of Jay W. Forrester to apply the **engineering principles of feedback and control** to **social systems**.

System Dynamics generates **qualitative models based on causalities**.

By appropriate parameterisation, the qualitative models can be transformed into “quantitative” **computer models to simulate** the investigated system

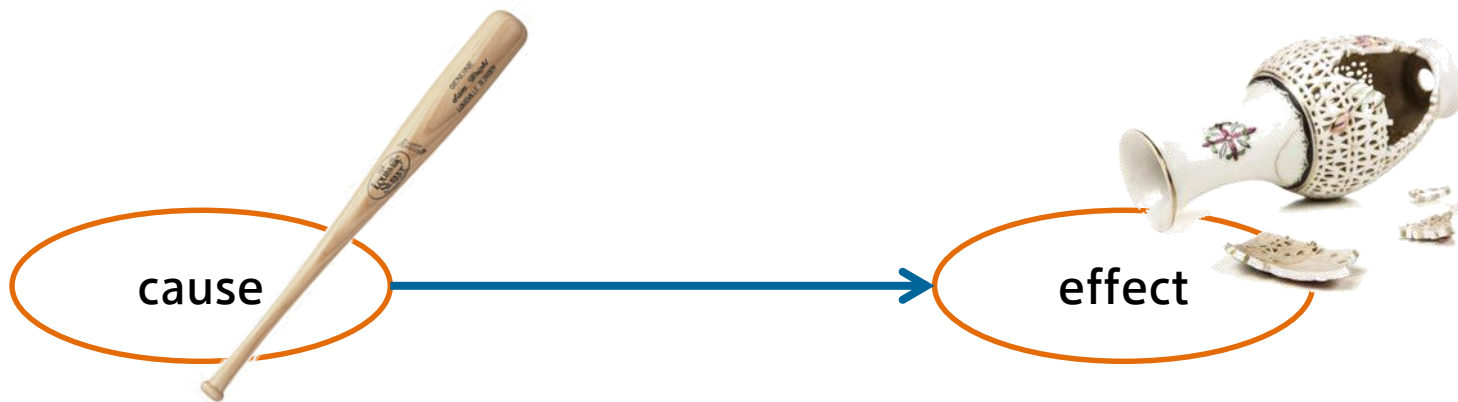
Systems Dynamics and **DYNAMO** received widespread interest mainly because they were used to build large world models such as

- WORLD2 (World Dynamics, Forrester 1971);
- WORLD3 (The Dynamics of Growth in a Finite World, [Meadows]);
- and WORLD3 revisited (Beyond the Limits).



Causal thinking is the key to organizing ideas in a system dynamics study

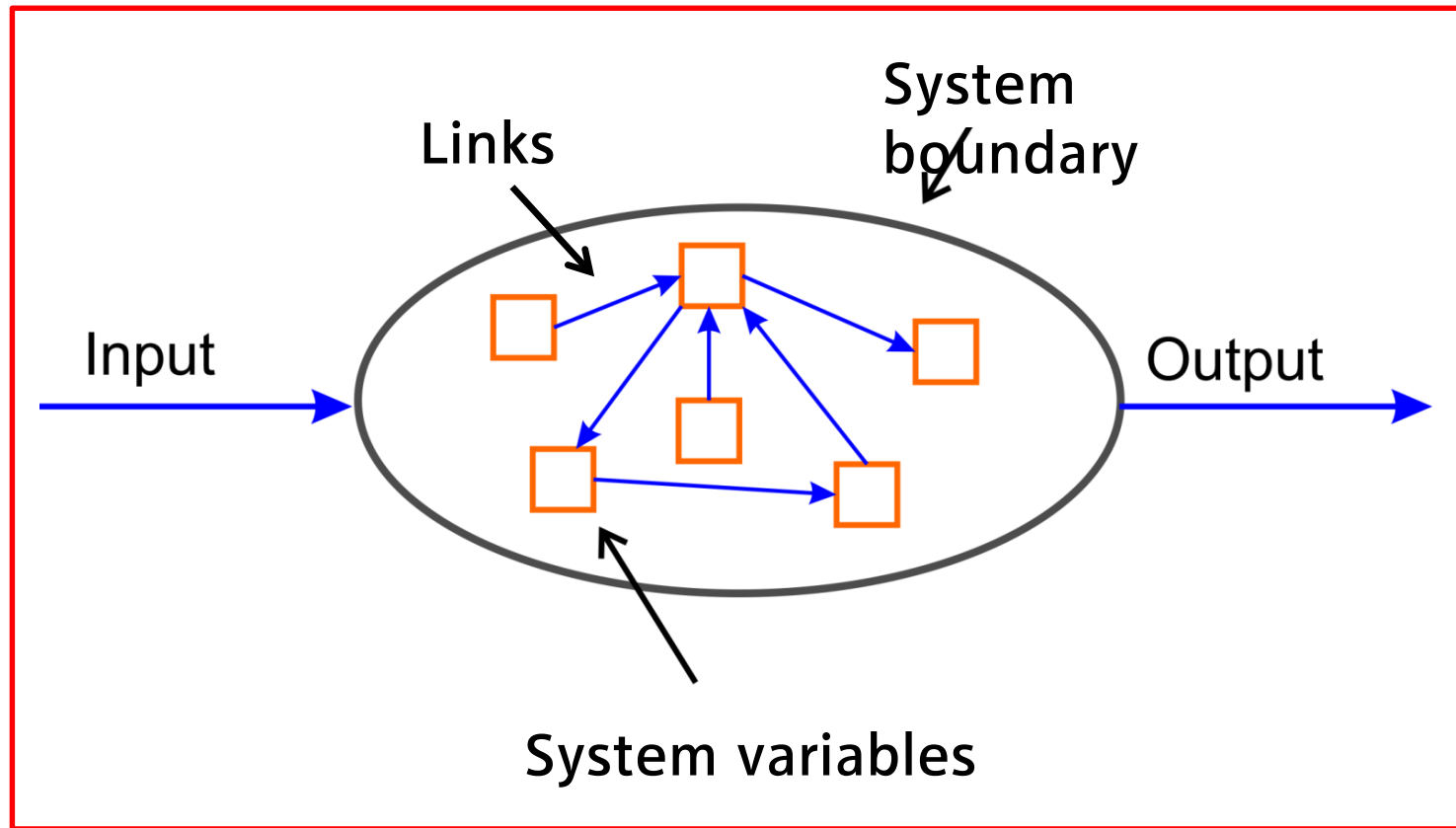
(Roberts et al. 1983)



1. Identify system variables and system boundaries
 2. Capture links of variables in a **Causal Loop Diagram (CLD)**
 3. Build a **Stock and Flow Diagram (SFD)**
-
- Implement the model in a simulator
-

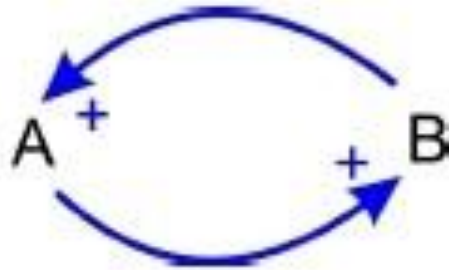
- a. Analysis of the problem - Determining the purpose and the use of the model and defining a target for the simulation.
 - b. Start collecting information and data. Start developing hypothesis about the parts of the system.
 - c. Determine the elements of the system.
 - d. Determine causal relationships between the elements.
-

1. System Variables and Boundaries



2. Causal Loop Diagram

Capture the **behavior** and **links** of and within the system by interlinking system variables that are related to each other



Behavior of system

- Feedback Loops
 - System memory (stocks)
 - Delays in material and information delays
-

2. Causal Loop Diagram

Main components of CLDs:

- **System variables:** names of elements
- **Link - positive:**



Represented by a plus-sign

Increase in variable *Eating* results in an increase in variable *Weight*

2. Causal Loop Diagram

Main components of CLDs:

- **Link – negative:**



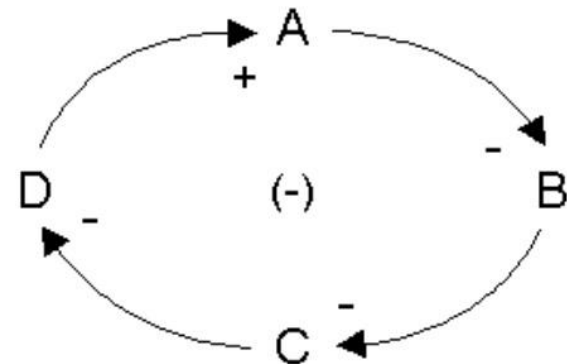
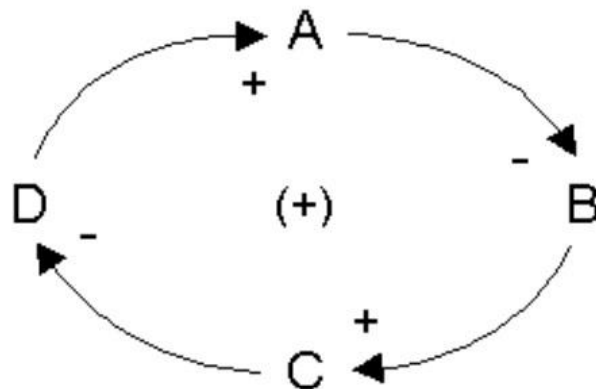
Represented by minus-sign.

Increase in variable *Diet* results in a decrease in variable *Weight*

2. Causal Loop Diagram

Main components of CLDs:

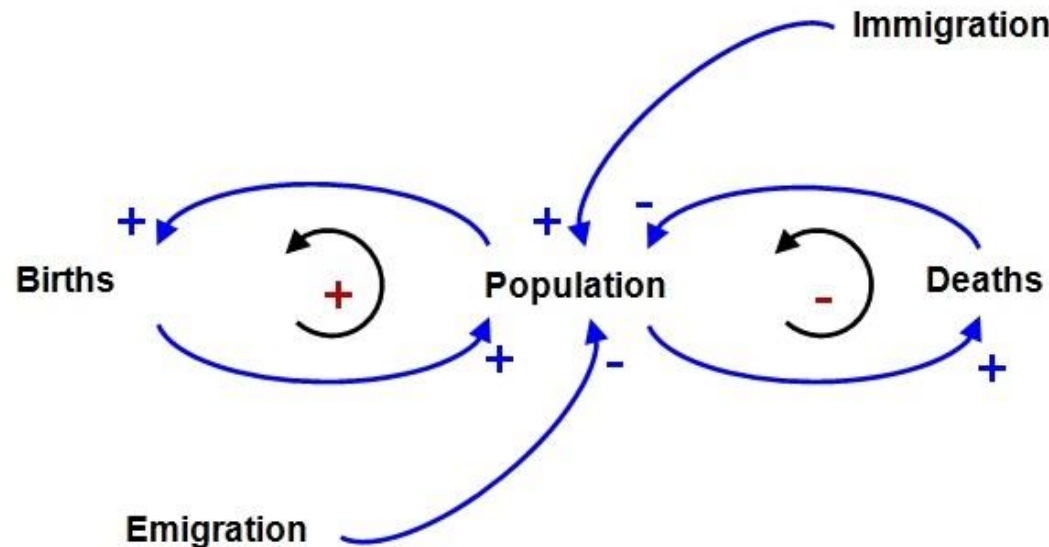
- **Feedback Loops:** are closed loops of arrows, represented by a:
“(+)” (or “(R)” for **reinforcing**) or
“(−)” (or “(B)” for **balancing**) sign in the middle.



2. Causal Loop Diagram

Main components of CLDs:

- **Feedback Loops:** are closed loops of arrows, represented by a “(+)” (or “(R)” for **reinforcing**) or “(-)” (or “(B)” for **balancing**) sign in the middle.



Feedback Loops

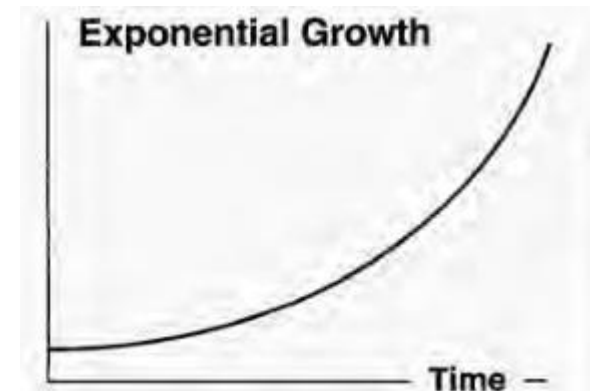
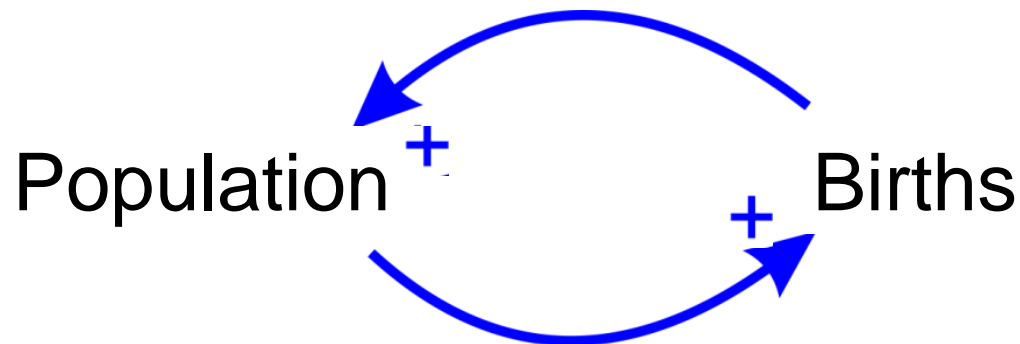
- Search to identify closed, causal feedback loops is one key element of System Dynamics
 - The most important causal influences will be exactly those that are enclosed within feedback loops
-

2. Causal Loop Diagram

Types of behavior due to loops:

- **Exponential Growth:** arises from **positive (reinforcing) feedback loop**.

Example:



2. Causal Loop Diagram

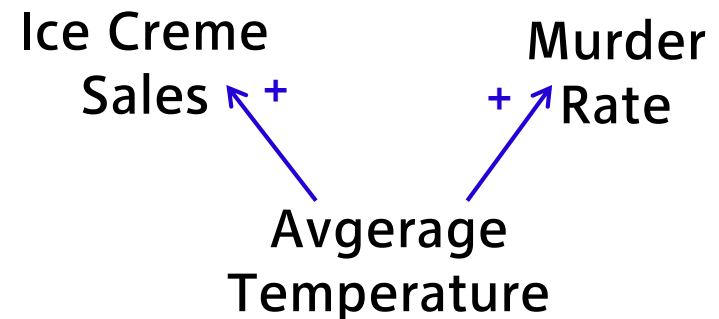
Causation vs. Correlation

- **Correlation** represents past behavior and not the structure of the system
- **Causation** represents the causal links of the structure

Wrong:

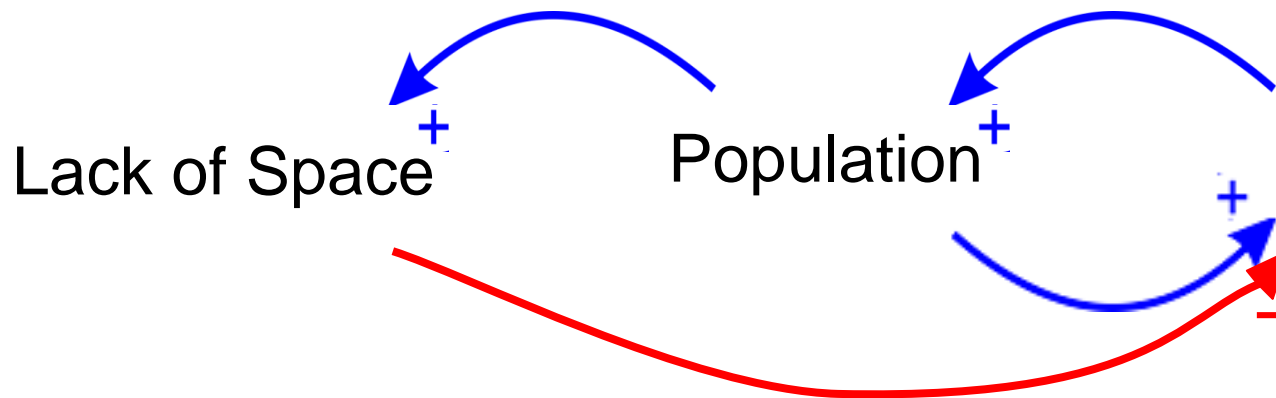


Right:



2. Causal Loop Diagram

At least one negative feedback loop is necessary to receive a stable system



Problem: Not all system elements are system variables!

Solution: distinguish between

- Sources/Sinks
 - Levels/Stocks
 - Flows
 - Auxiliaries
 - Parameters
 - Links
-

Sources/Sinks:



Source represents systems of levels and rates outside the boundary of the model

Sink is where flows terminate outside the system

E.g.: Raw Material (Source for „Construction“ Flow), Graveyard (Sink for „Dying“ Flow)

Levels/Stocks/System variables:

A quantity that accumulates over time and changes its value continuously.



E.g.: Size of a population, Number of people waiting in a queue, Number of goods waiting to be transported, etc.

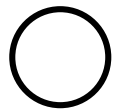
Flow/Rate/Activity/Movement:



Changes the values of levels. Every level has at least to be connected to one flow in order to change its value.

E.g.: Birth (Changes the value of the stock „population“), Eating (Changes the value of the stock „amount of food“), etc.

Auxiliary:



Everything that can directly/analytically be calculated out of stocks and constants.
Often useful, to avoid confusing models.

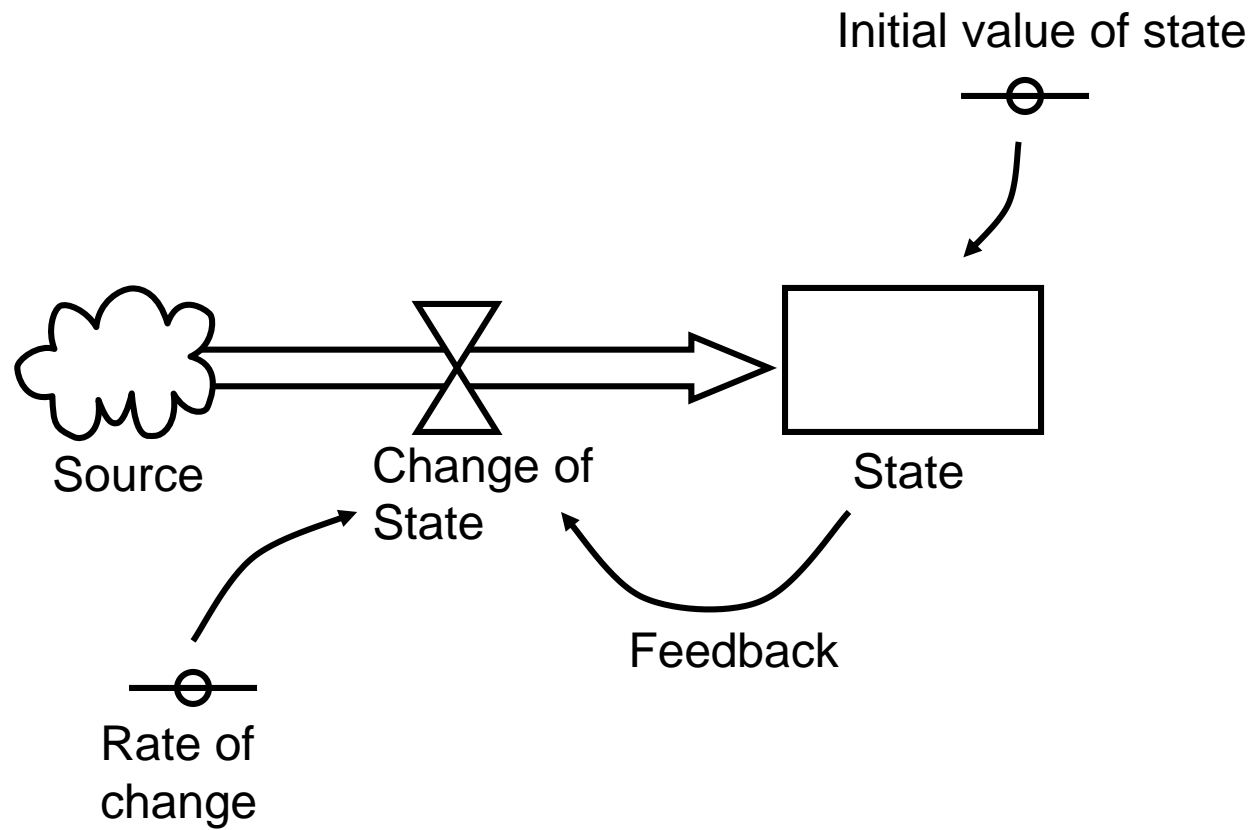
E.g.: Density (can directly be calculated by the stocks/constants „mass“ and „volume“), Queue length (calculated by stock „people in queue“ and constant „average size of one person“), etc.

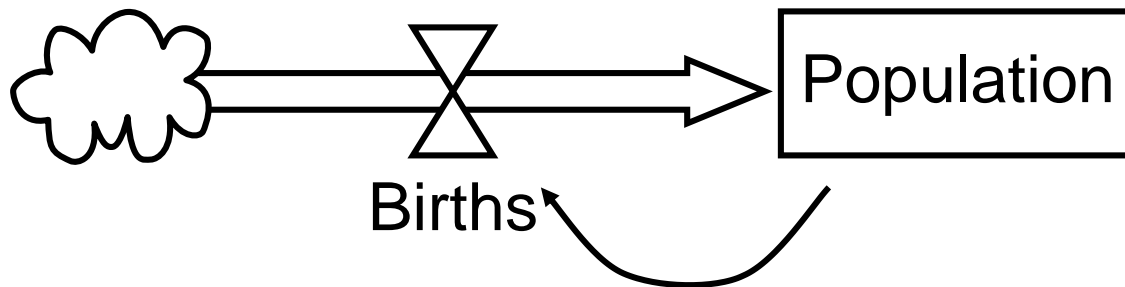
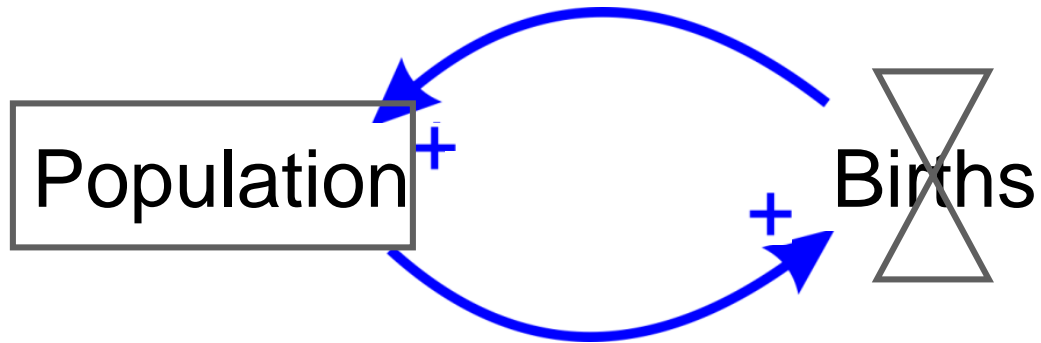
Parameter /Constant

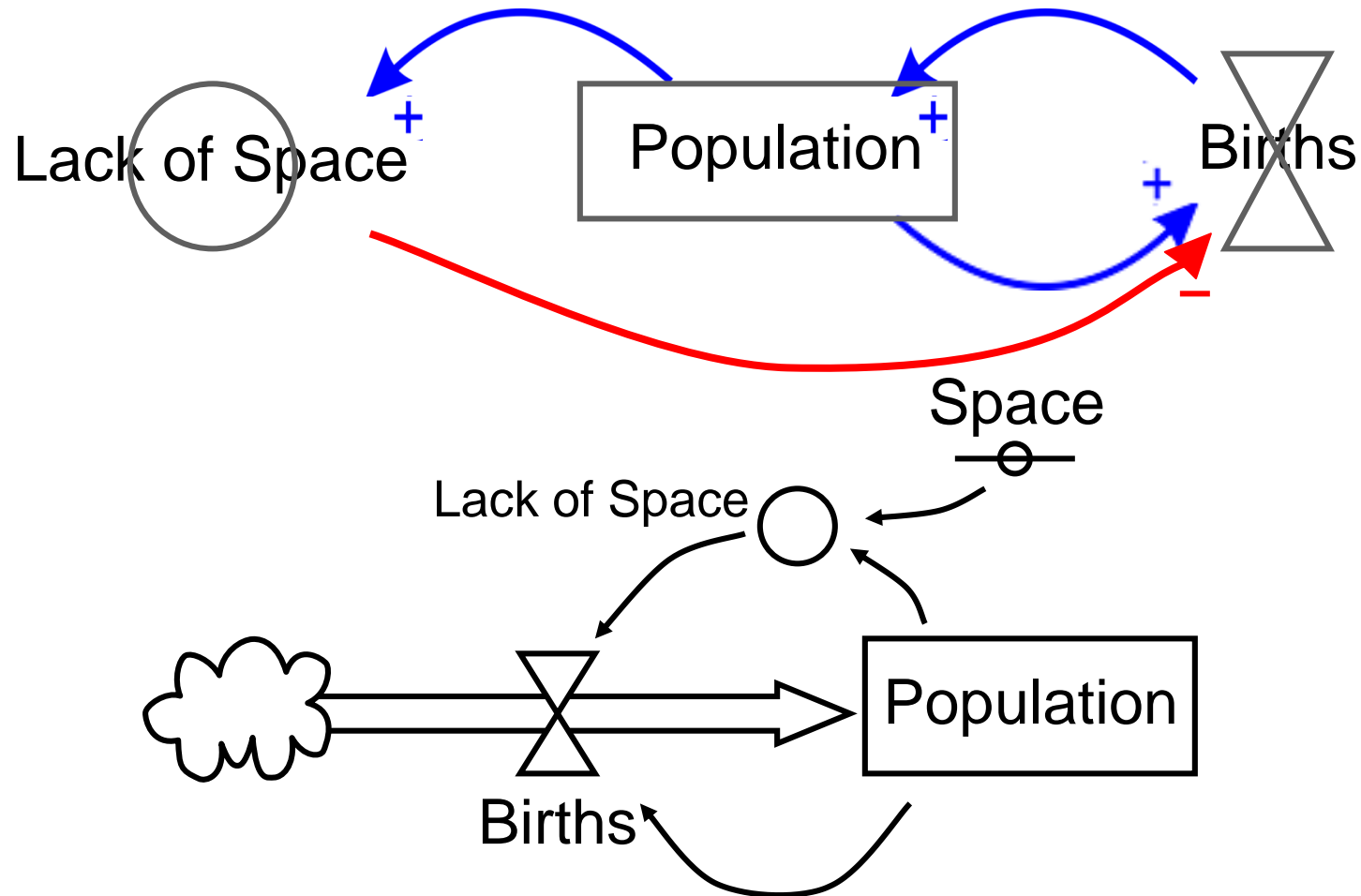


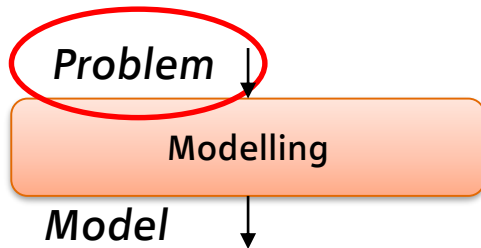
Everything that is predefined for the whole simulation – usually it is a constant but can be a function too.

E.g.: Average Temperature, Number of Cash Desks (In a supermarket), Birth Rate, Maximum capacity of a Room, etc.









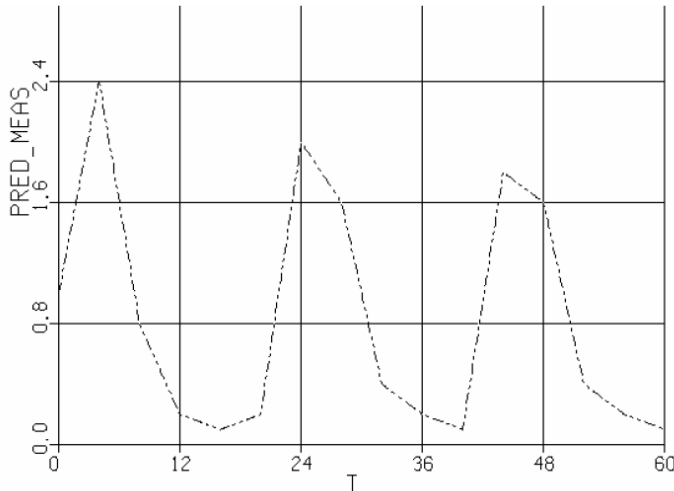
Dynamics: Predator eats Prey
Predator / Prey births, deaths



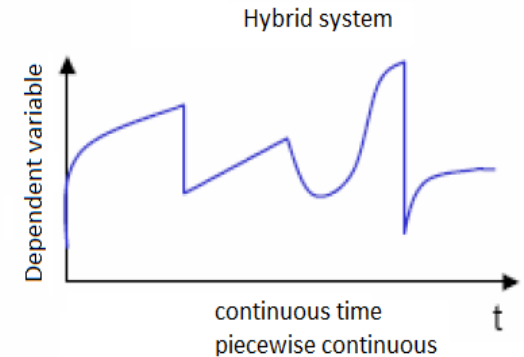
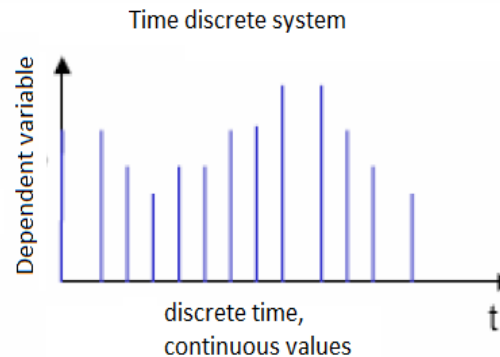
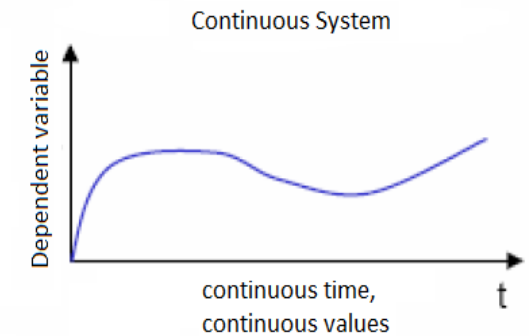
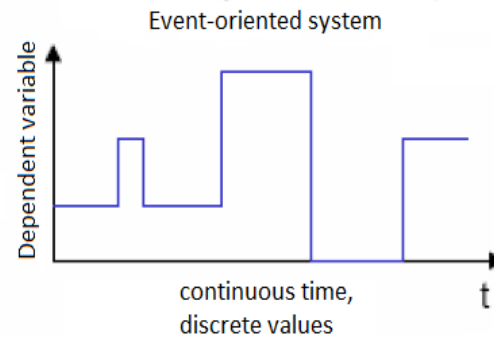
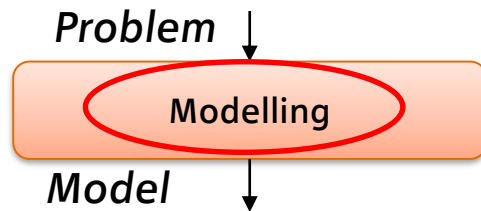
Environment: isolated

Measurement: Predator Population
5 Years = 60 months, quarterly

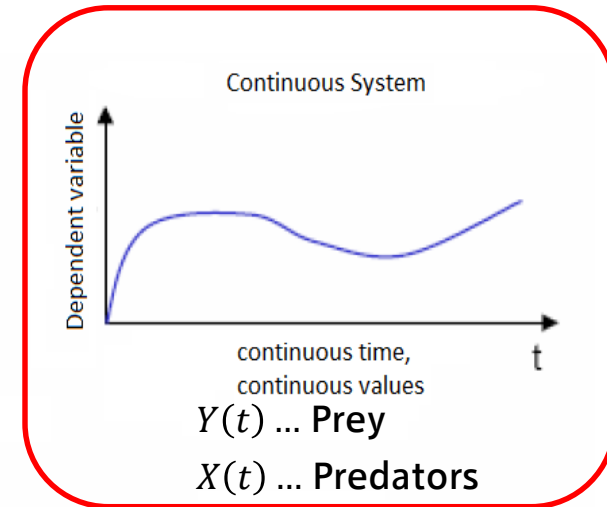
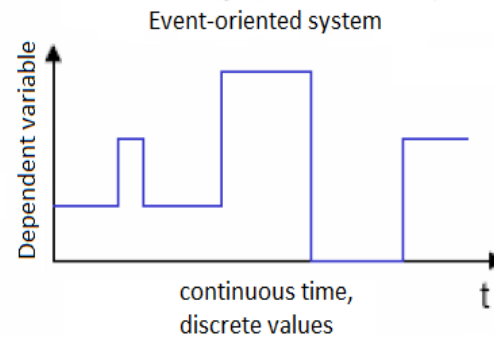
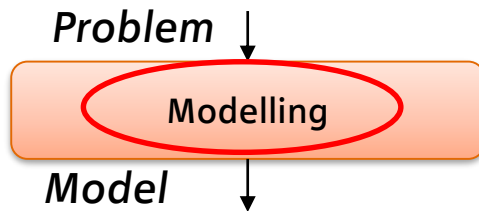
Problem: When is a reasonable time to use chemical pesticides to reduce number of predators?



Predator – Prey System

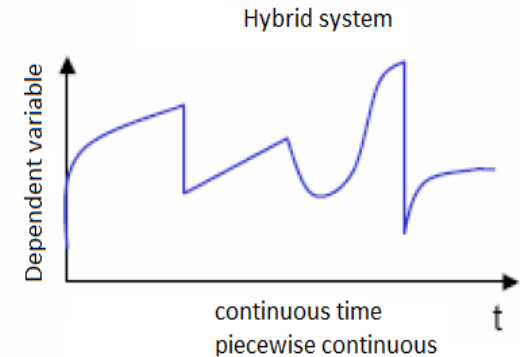
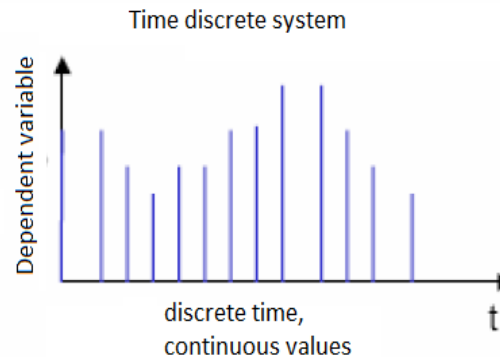


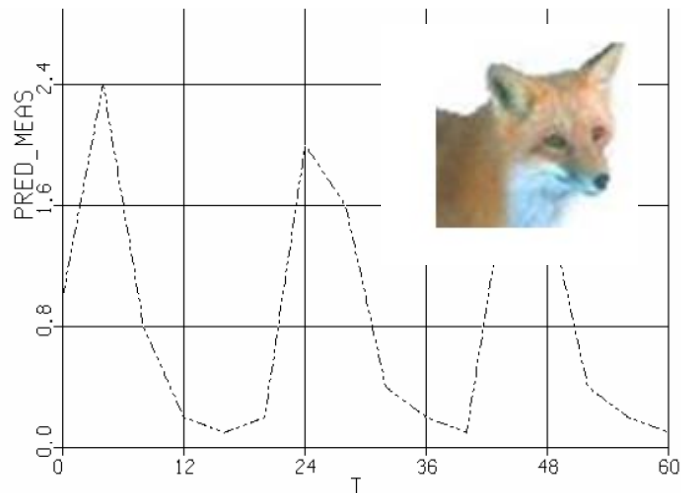
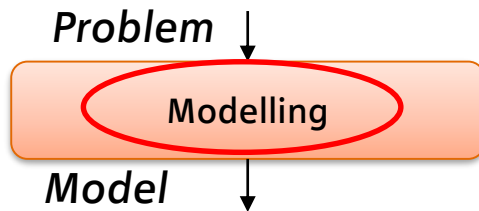
Predator – Prey System



Separation –
Isolated environment

Choice -
2 variables = 2 states





Separation -

Isolated environment

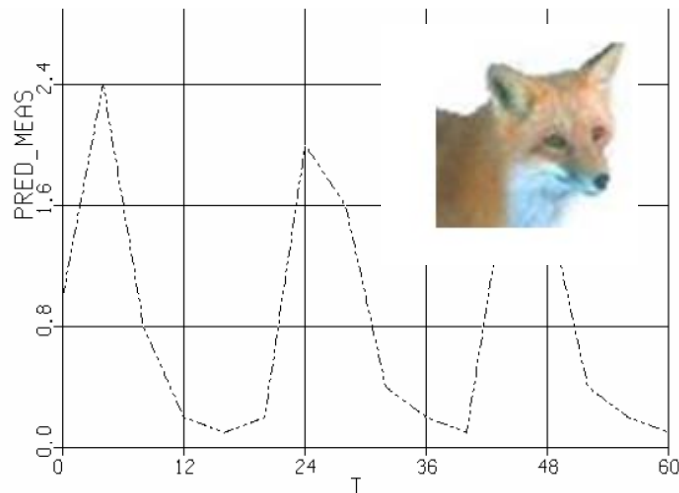
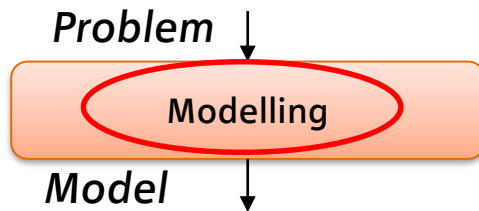
Choice -

2 variables = 2 states

Causality -

Predator - Prey - Model





Separation -

Isolated environment

Choice -

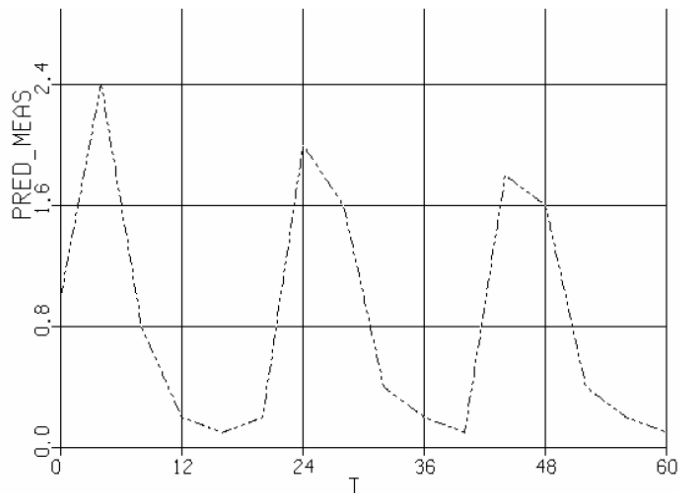
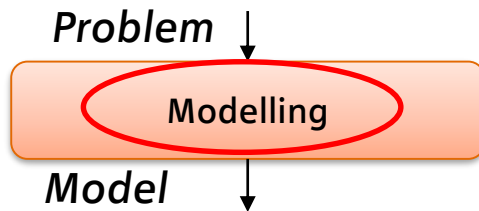
2 variables = 2 states

Causality -

Predator – Prey – Model

$Y(t)$.. Prey Population

$X(t)$.. Predator Population



Causality -

Predator - Prey - Model

$Y(t)$.. Prey Population

$X(t)$.. Predator Population

System Dynamics -

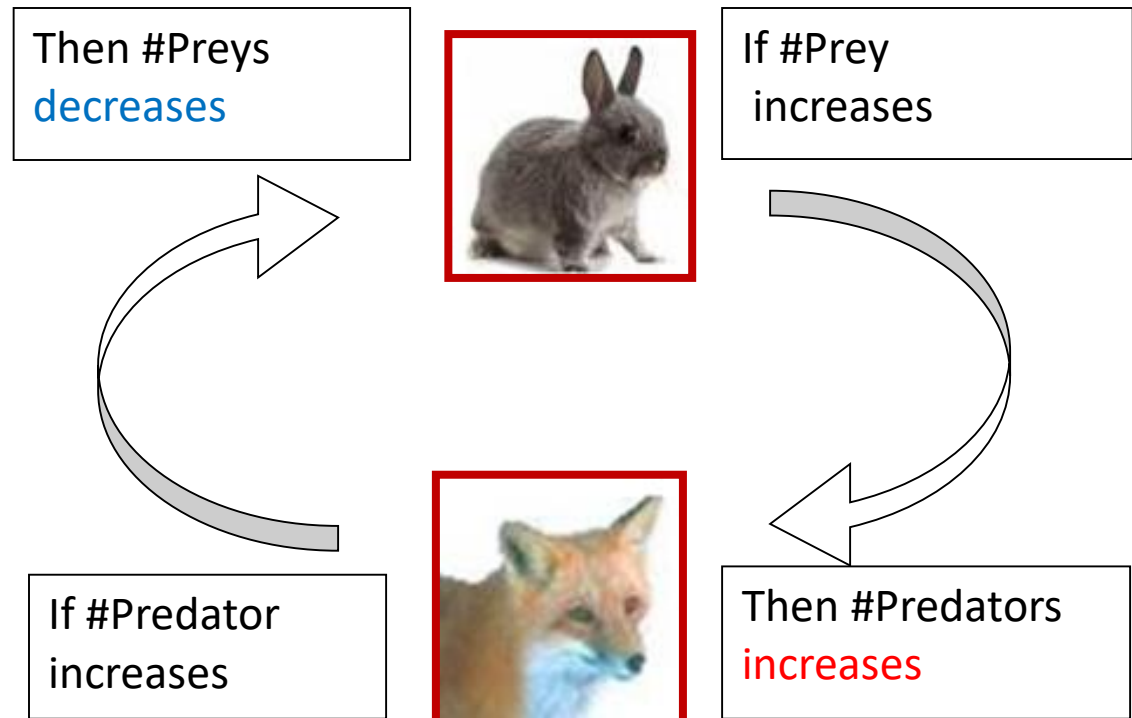
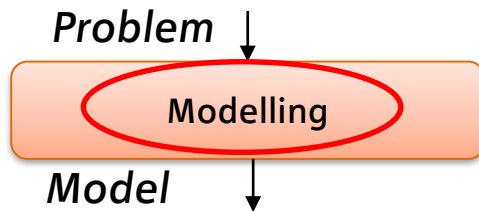
Population Interaction

Causality – Predator – Prey – Model

$Y(t)$.. Prey,

$X(t)$.. Predator

System Dynamics - Population interaction

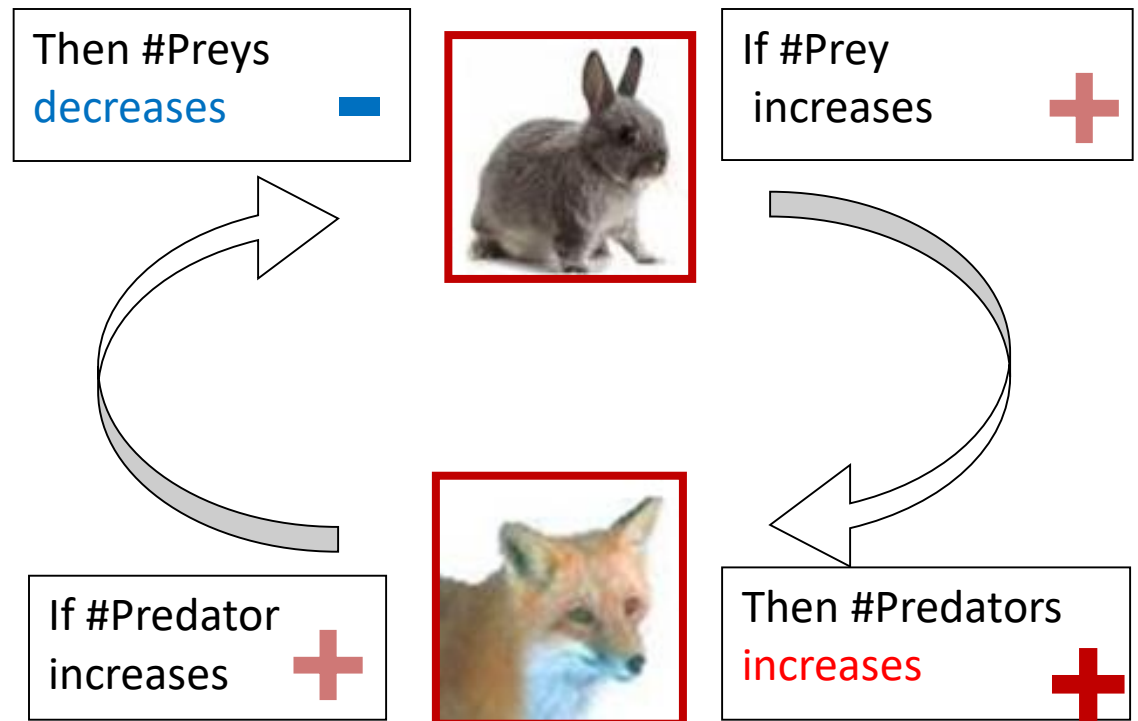
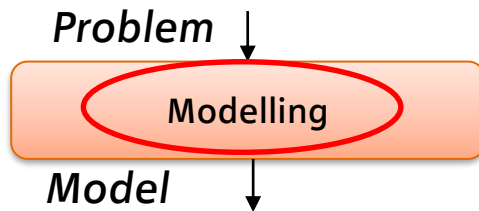


Causality – Predator – Prey – Model

$Y(t)$.. Prey,

$X(t)$.. Predator

System Dynamics - Population interaction

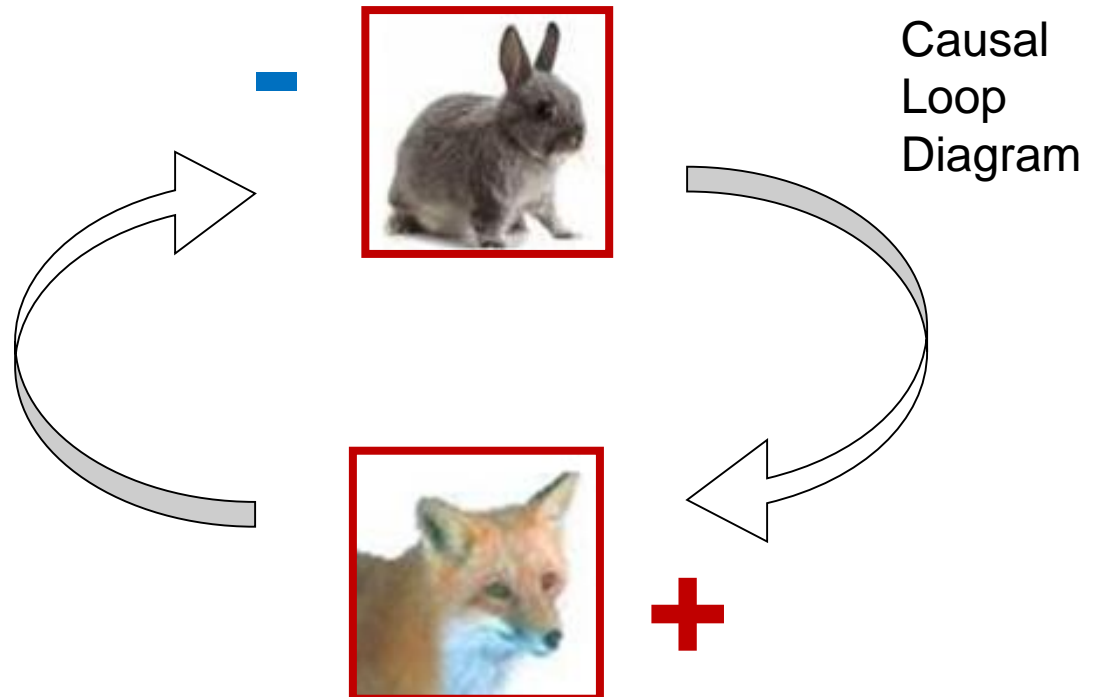
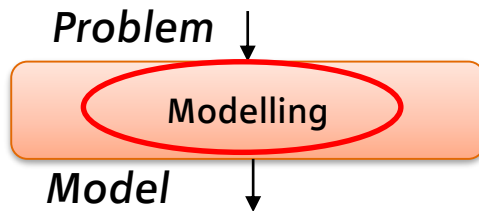


Causality – Predator – Prey – Model

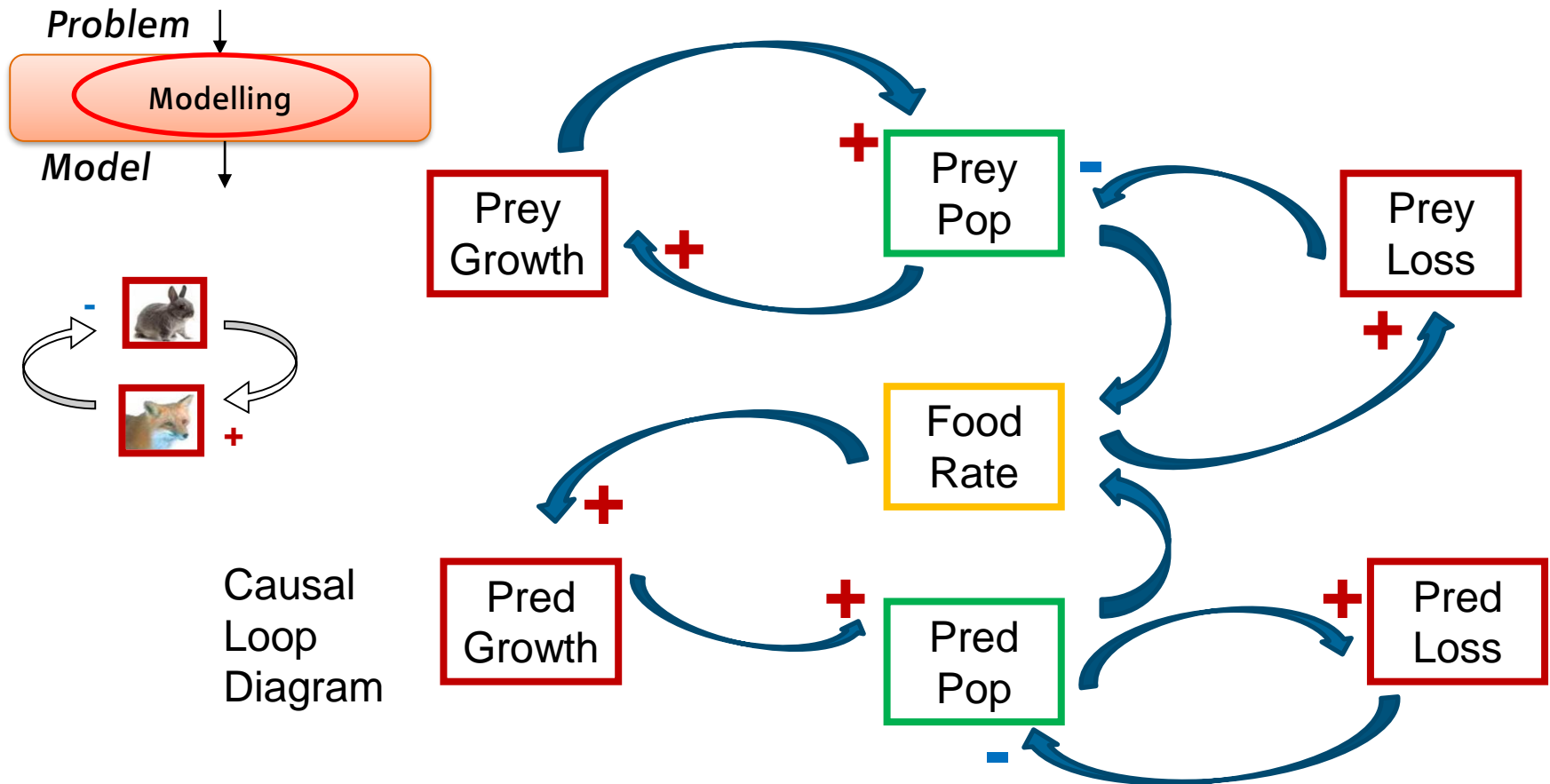
$Y(t)$.. Prey,

$X(t)$.. Predator

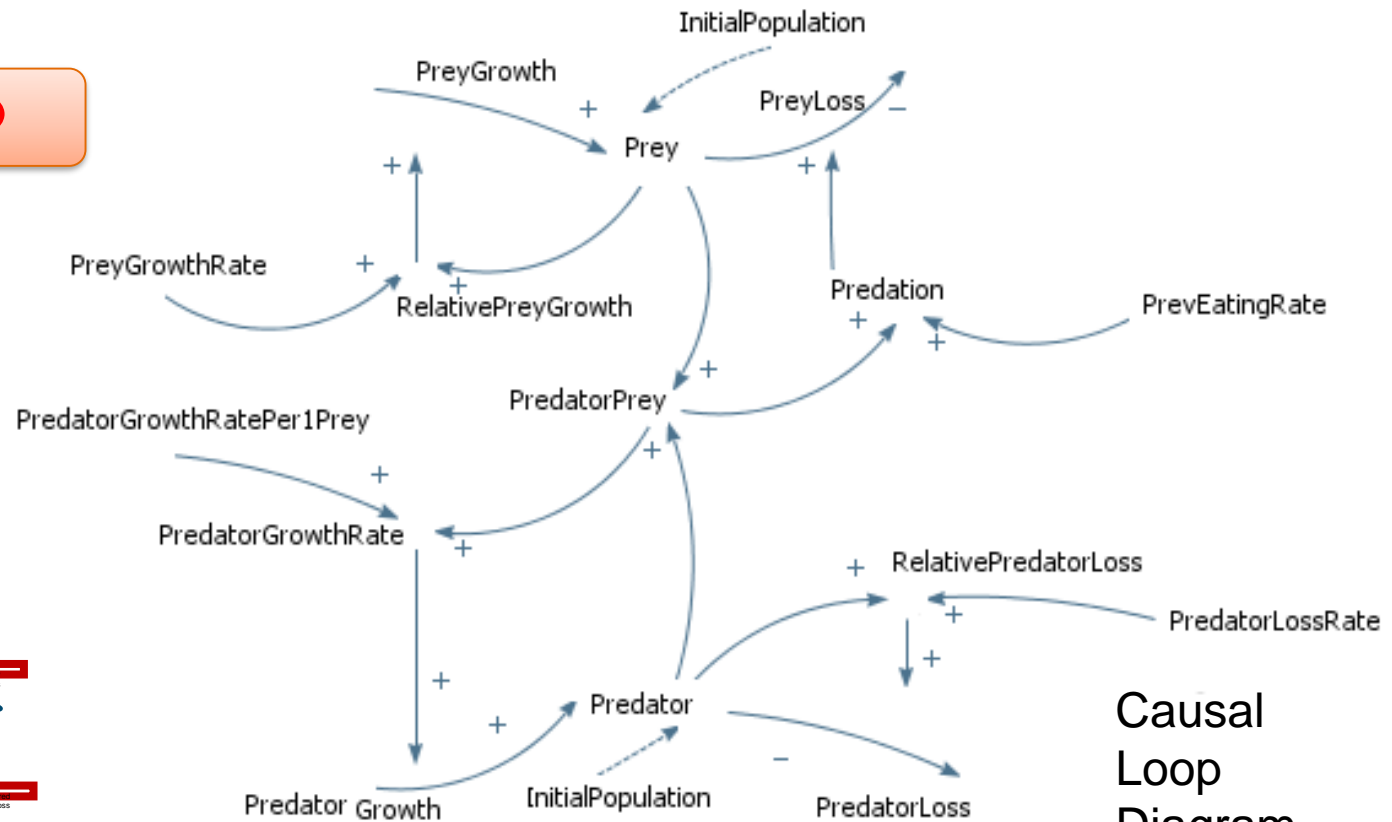
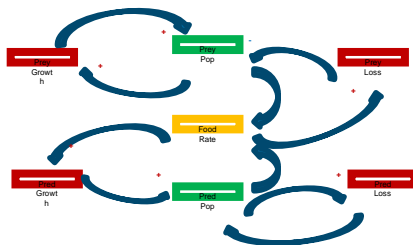
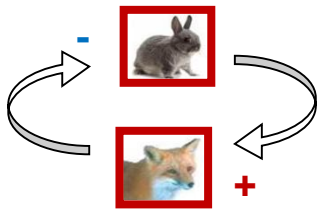
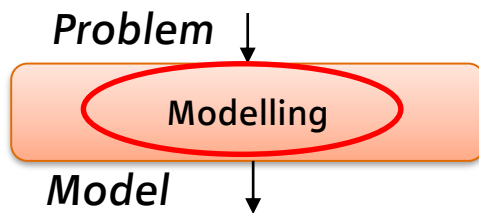
System Dynamics - Population interaction



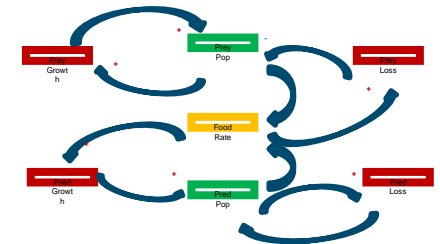
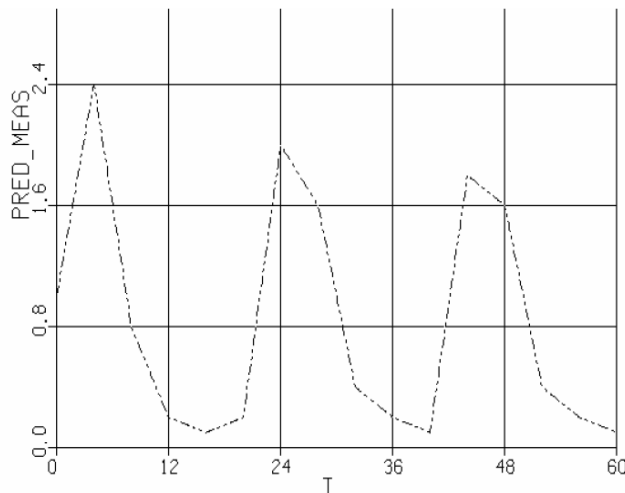
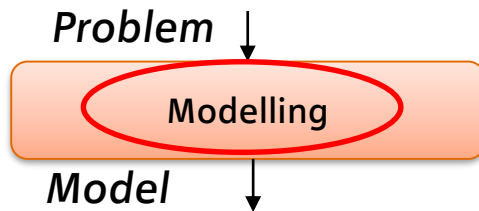
System Dynamics - Population interaction



System Dynamics - Population interaction



Causal Loop Diagram



Causality –

Predator – Prey – Model

$x(t)$.. Prey

$y(t)$.. Predator

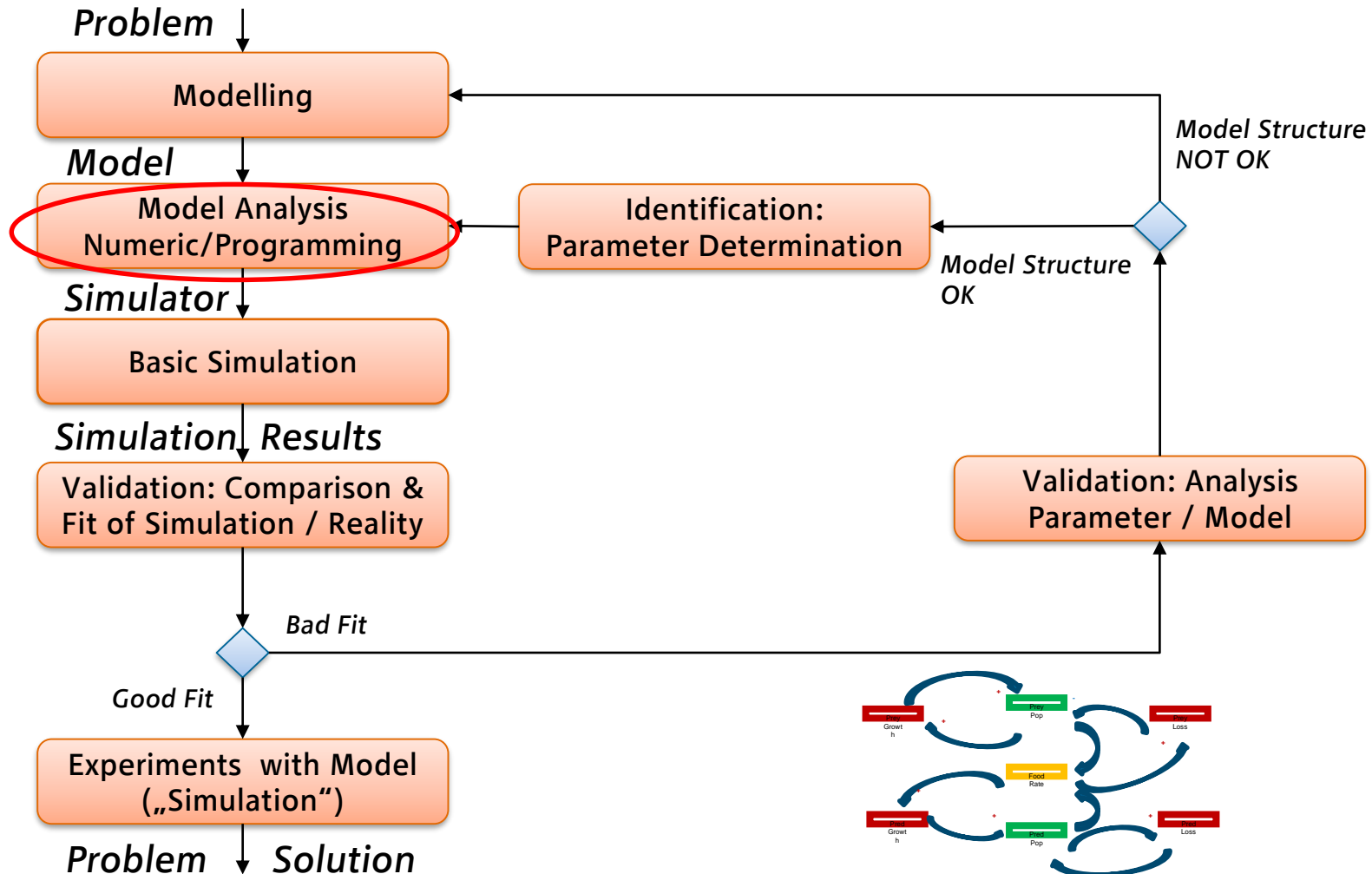
Logistic Growth –

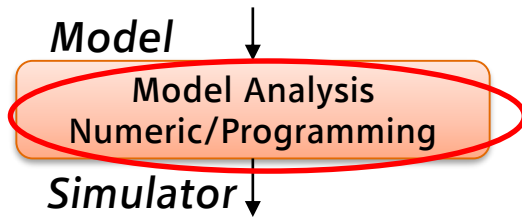
$$\dot{x} = ax - bxy$$

$$\dot{y} = -dy + exy$$

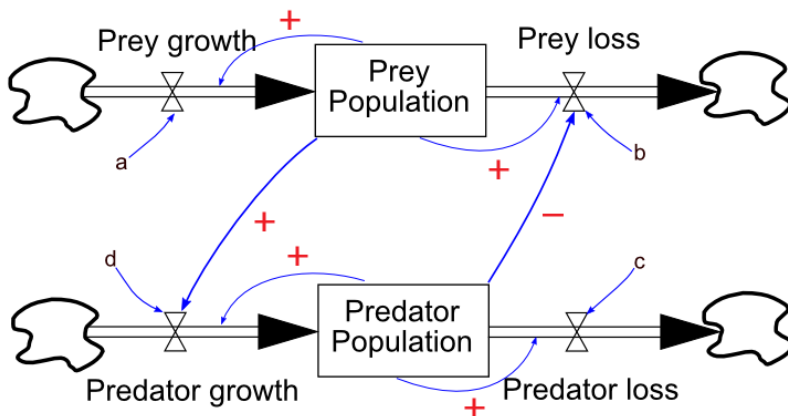
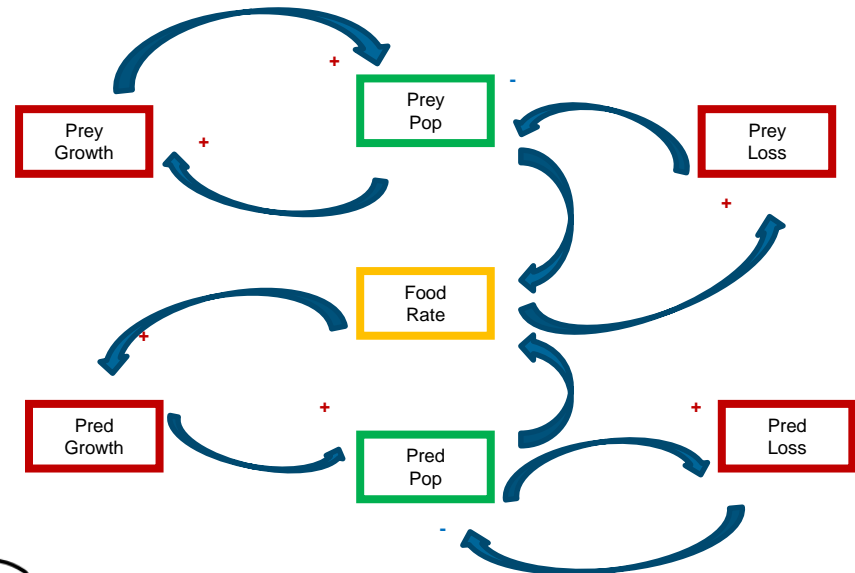
Population rate = Growth rate + food rate

Simulation Circle: Predator - Prey

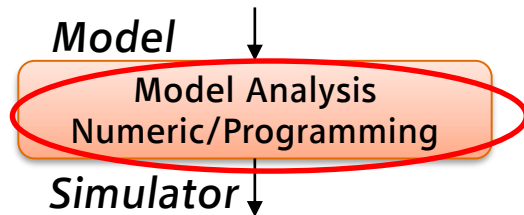




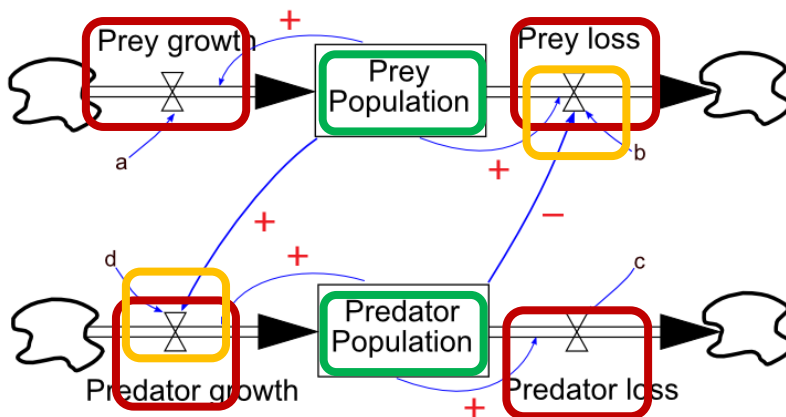
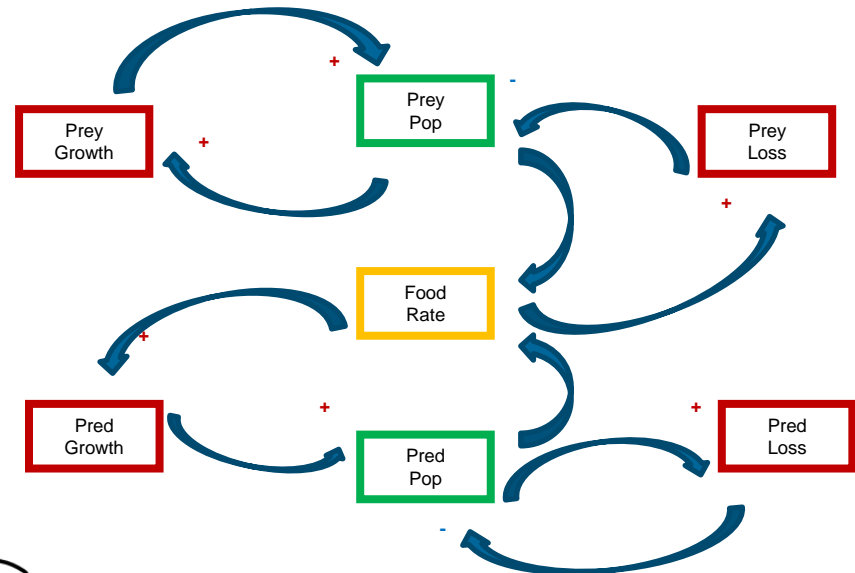
Causal Loop Diagram



Stock and Flow Diagram

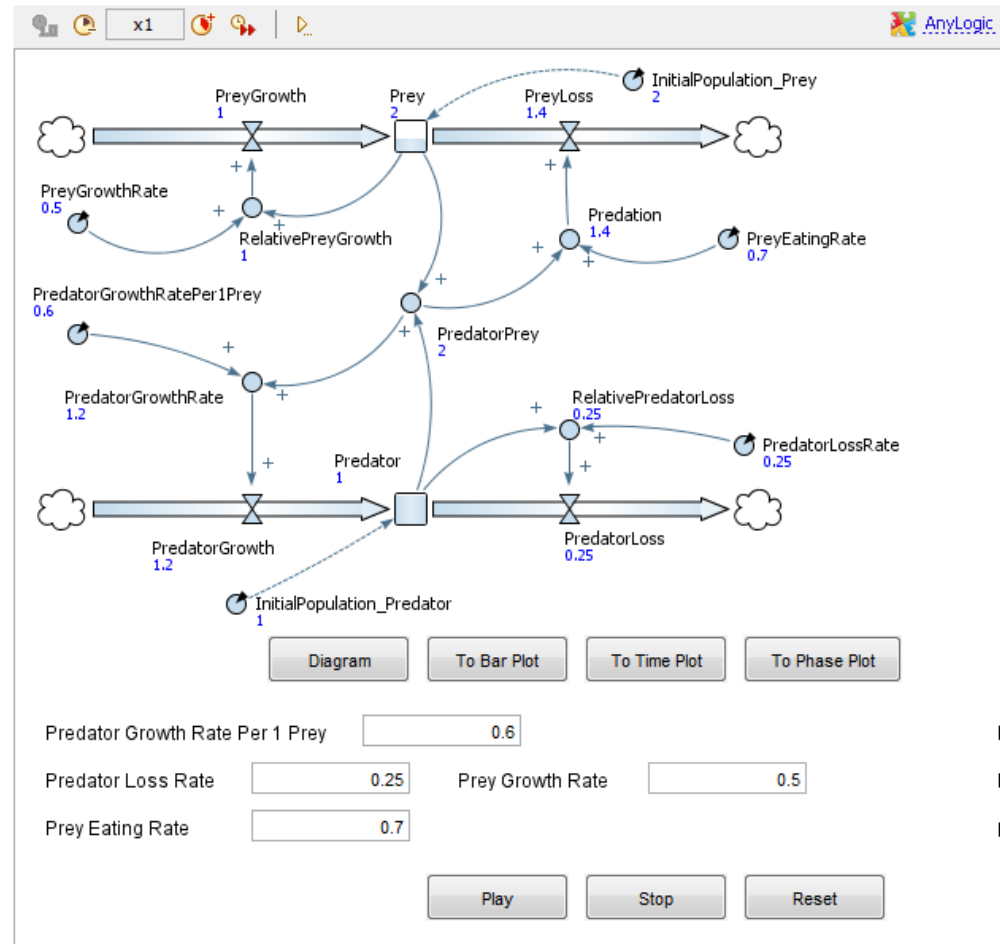
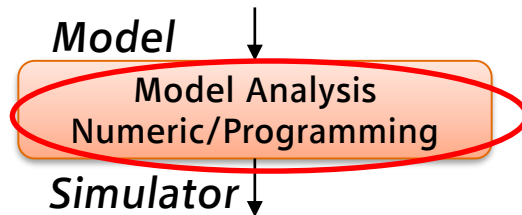


Causal Loop Diagram

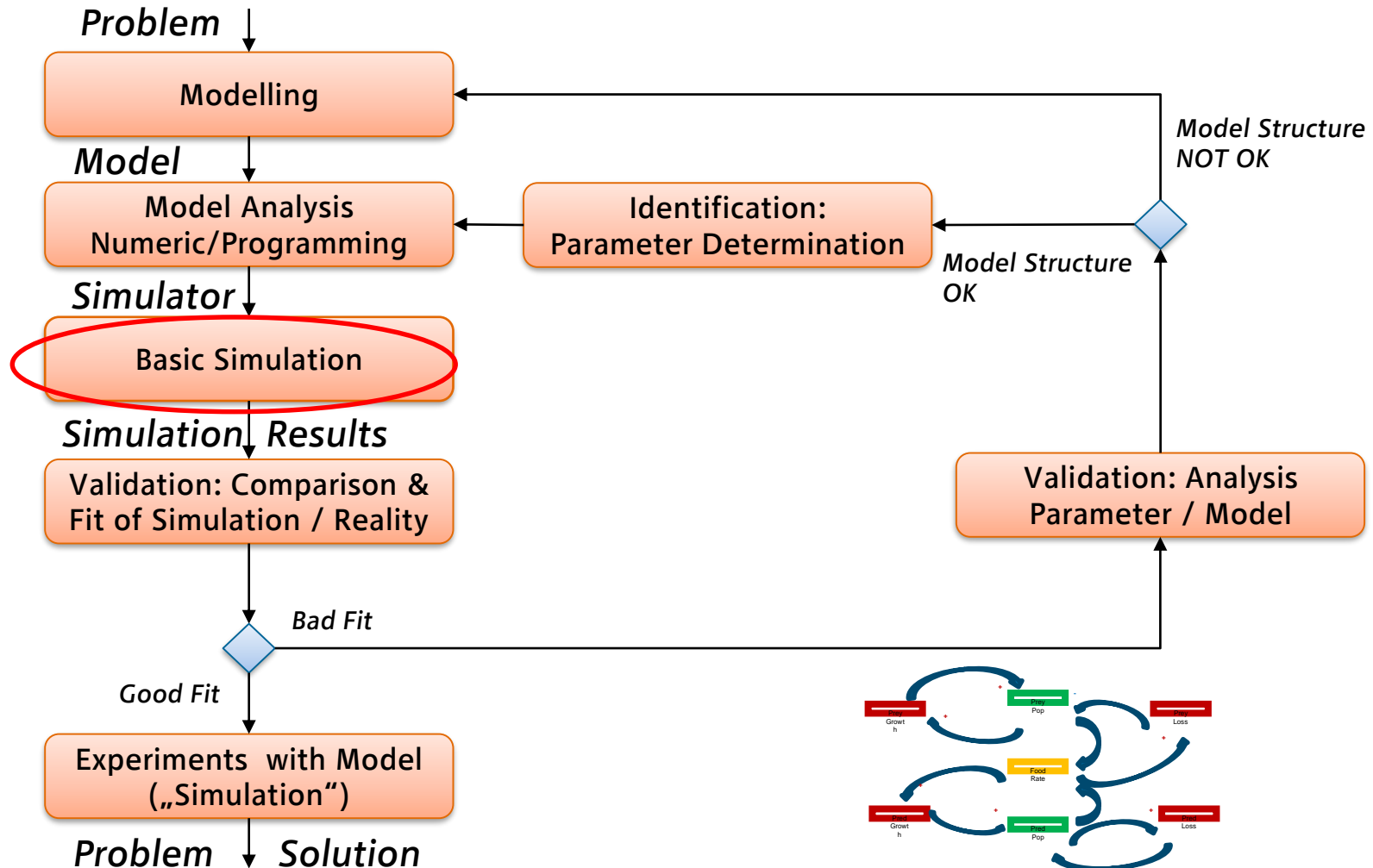


Stock and Flow Diagram

Implementation



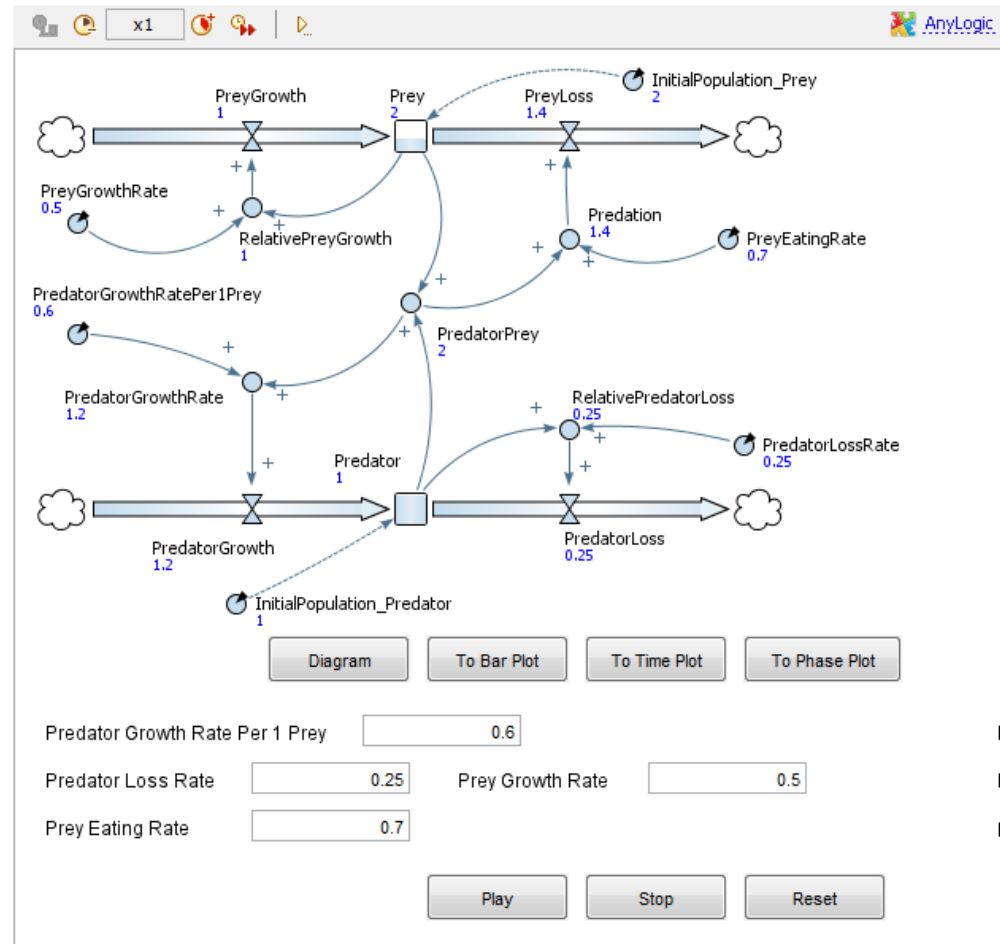
Simulation Circle: Predator - Prey



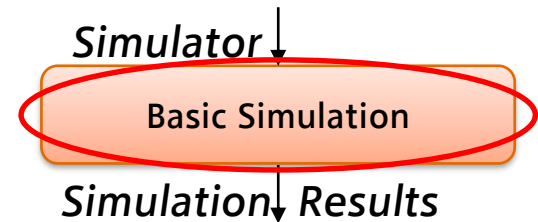
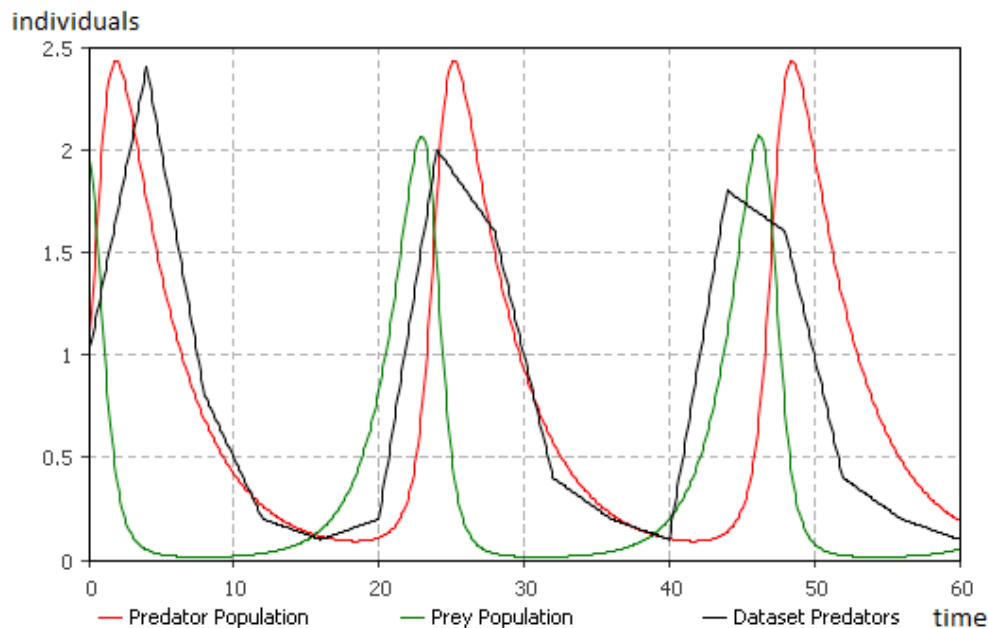
Simulator

Basic Simulation

Simulation Results



Population development over time:



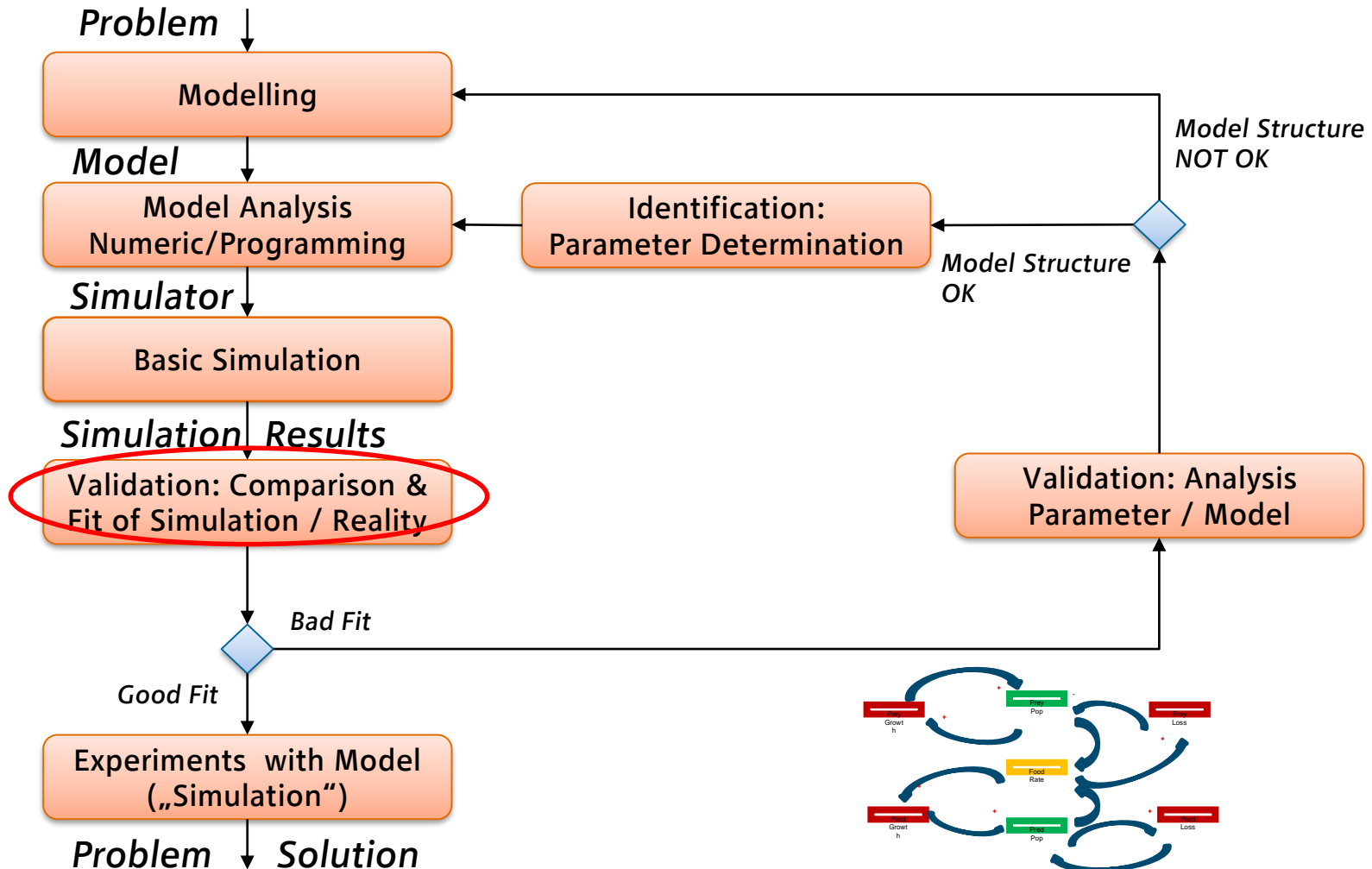
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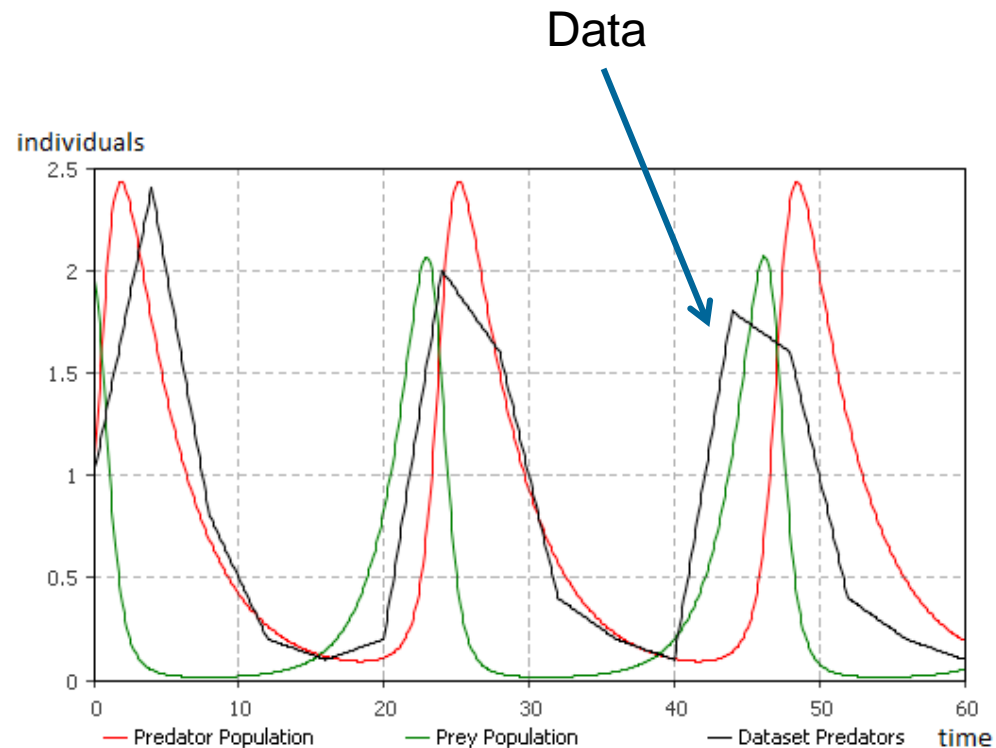
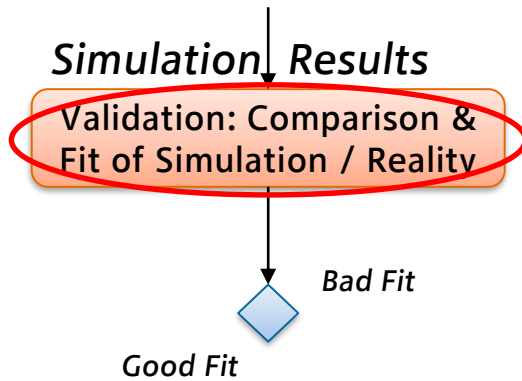
Predator Growth Rate Per 1 Prey	<input type="text" value="0.6"/>
Predator Loss Rate	<input type="text" value="0.25"/>
Prey Eating Rate	<input type="text" value="0.7"/>
Prey Growth Rate	<input type="text" value="0.5"/>

$$\dot{x} = (a - b \cdot y)x$$

$$\dot{y} = (-c + d \cdot x)y$$

Simulation Circle: Predator - Prey





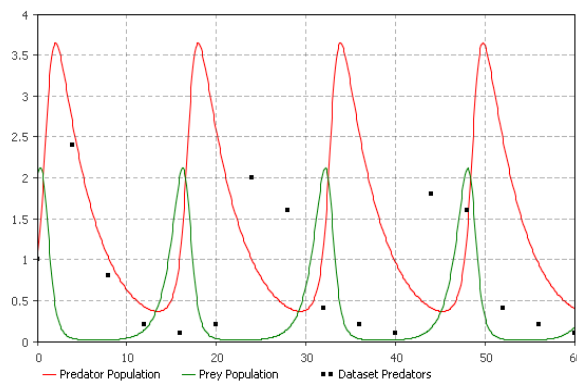
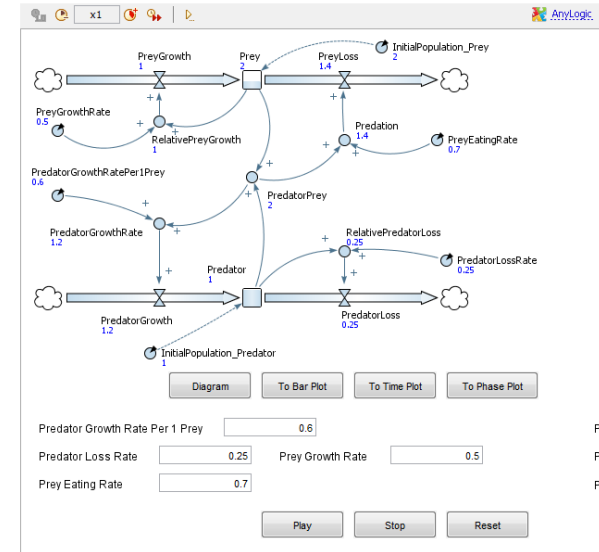
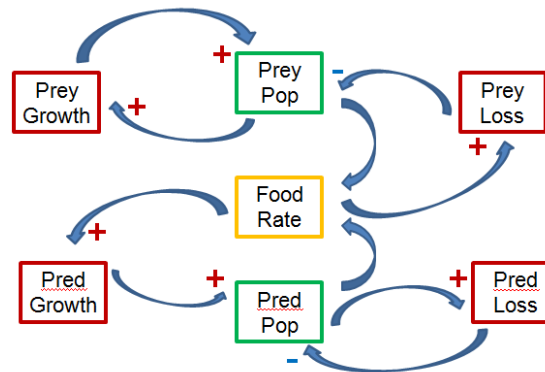
Data & Simulation Results

Simulation Results

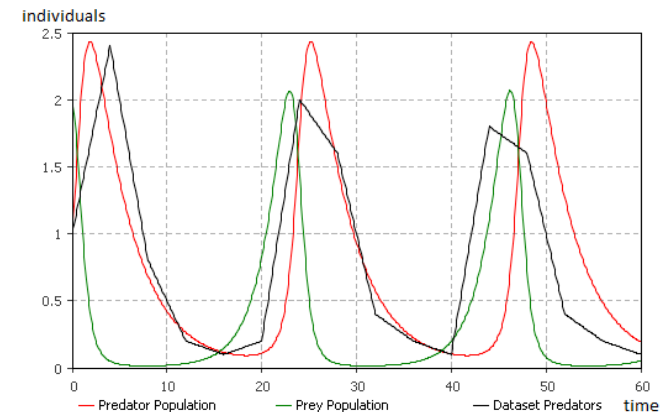
Validation: Comparison & Fit of Simulation / Reality

Bad Fit

Good Fit



Search for
convenient
parameters



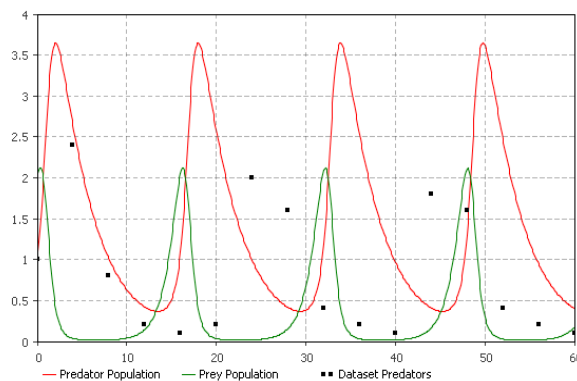
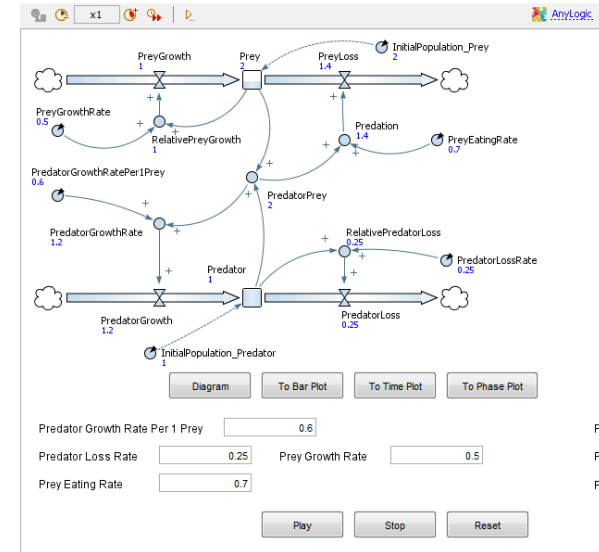
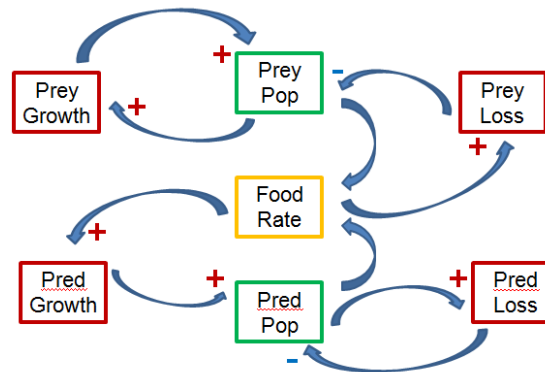
Data & Simulation Results

Simulation Results

Validation: Comparison & Fit of Simulation / Reality

Bad Fit

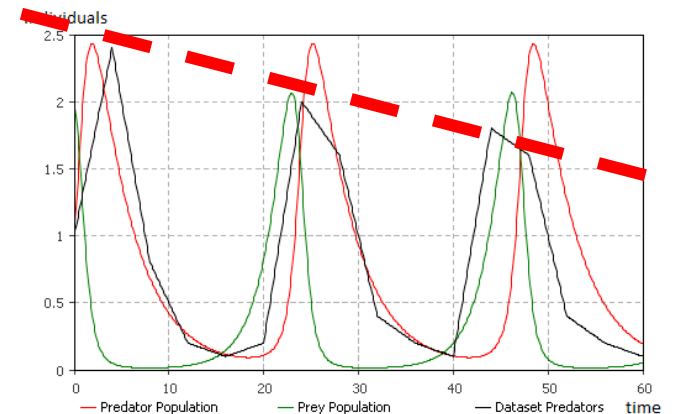
Good Fit



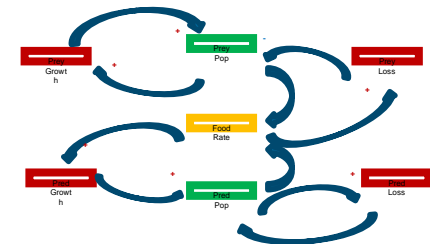
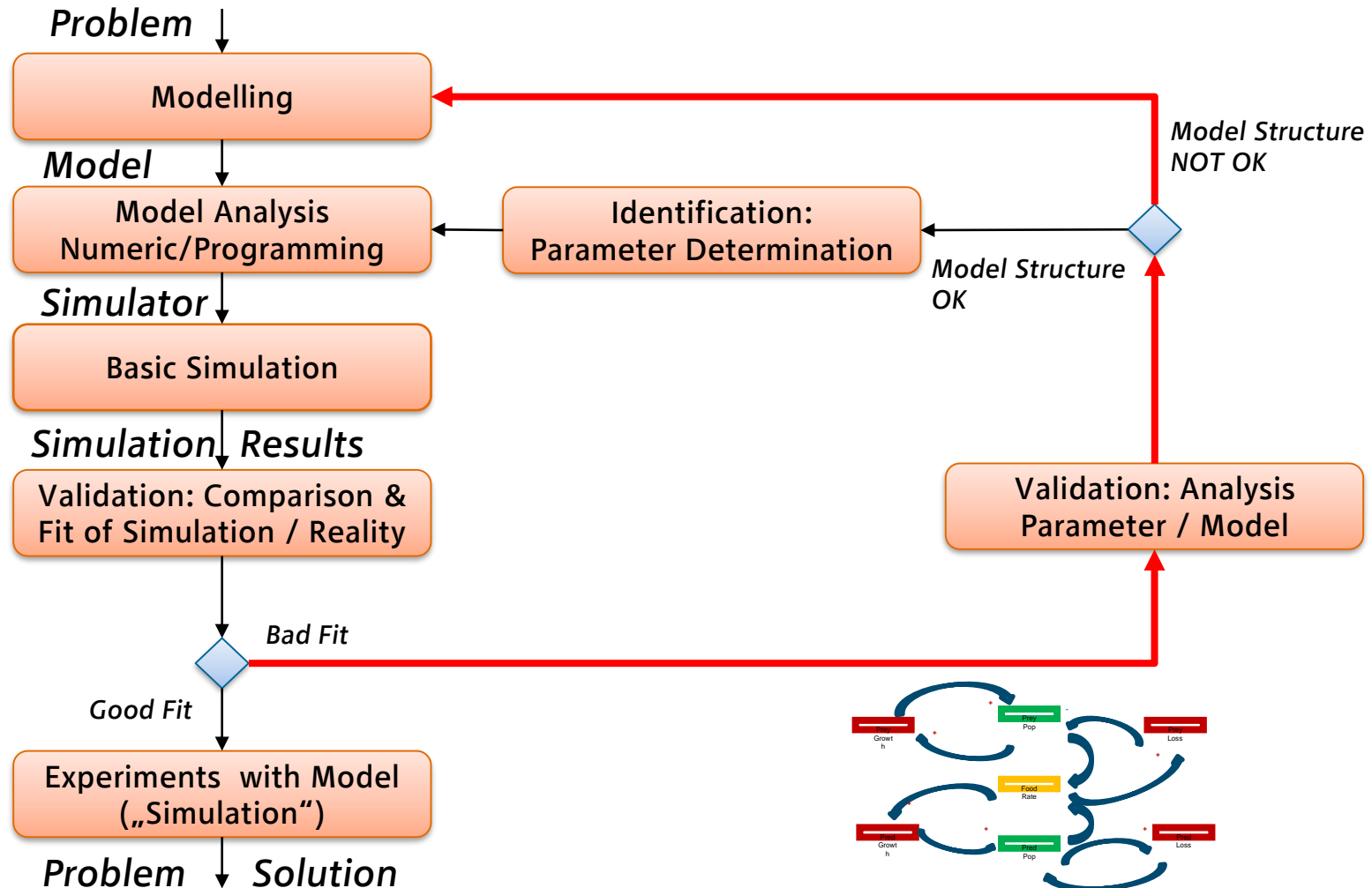
Search for
convenient
parameters

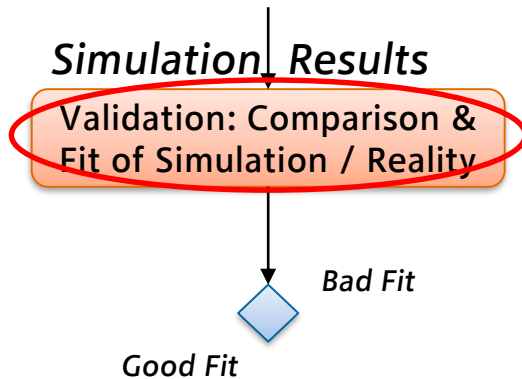


No
Damping
in Model



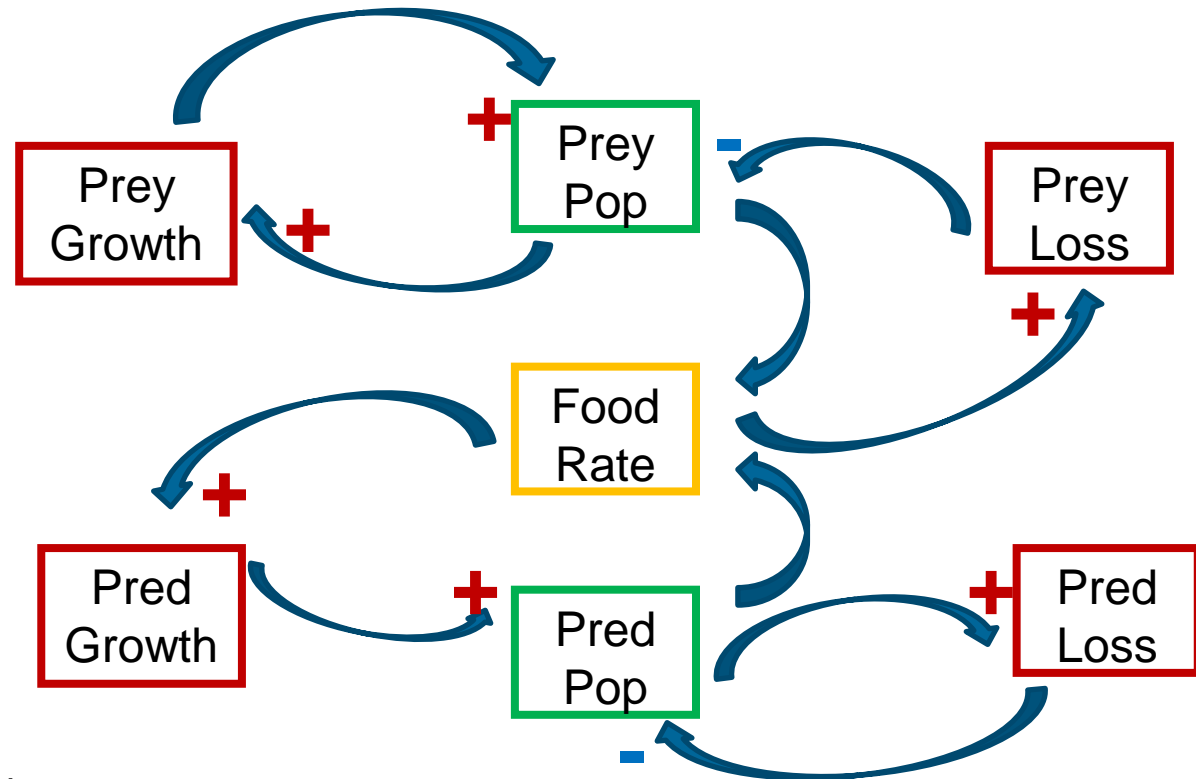
Simulation Circle: Predator - Prey

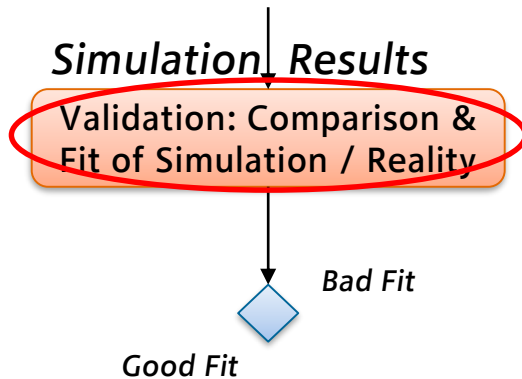




Model Extension:

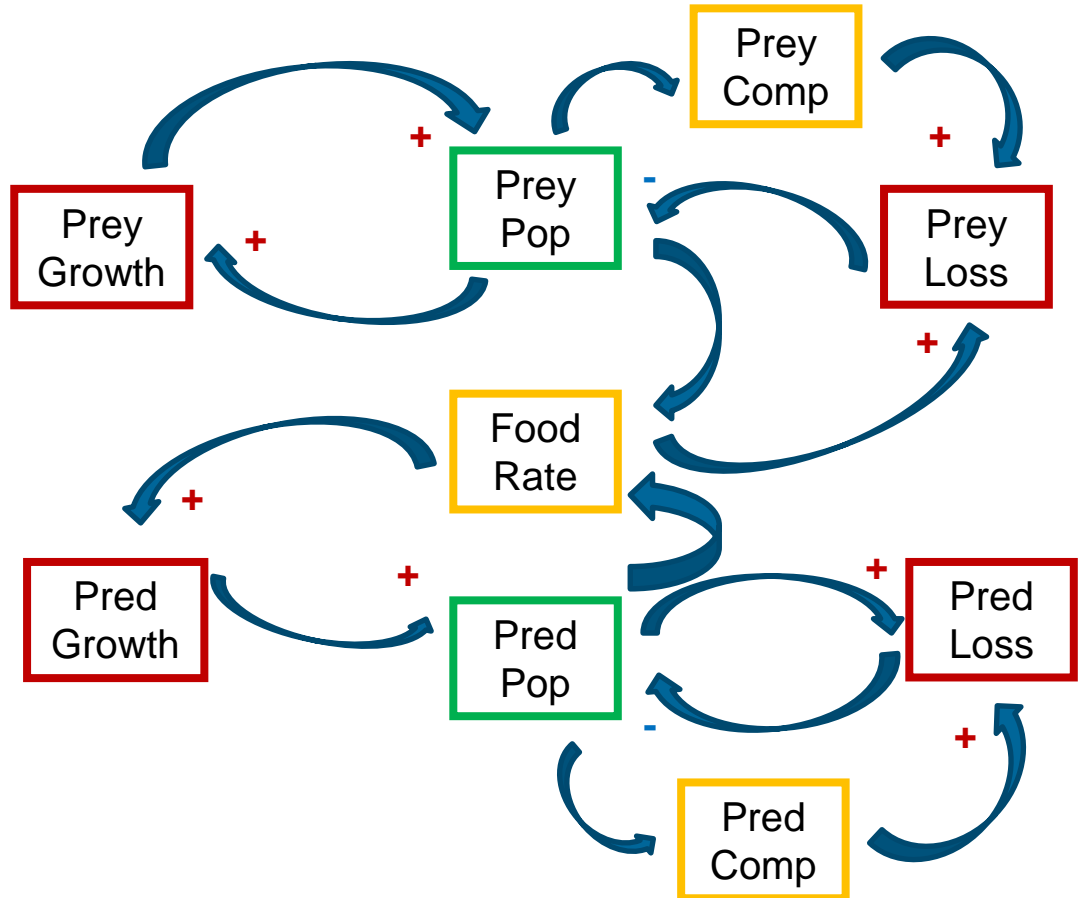
- Both the predator and the prey compete for food and shelter in the forest.
- Competition sets in and the population of each species tends to control itself via a negative effect, that is the population decreases with a rate directly proportional to the present population of that species.





Model Extension:

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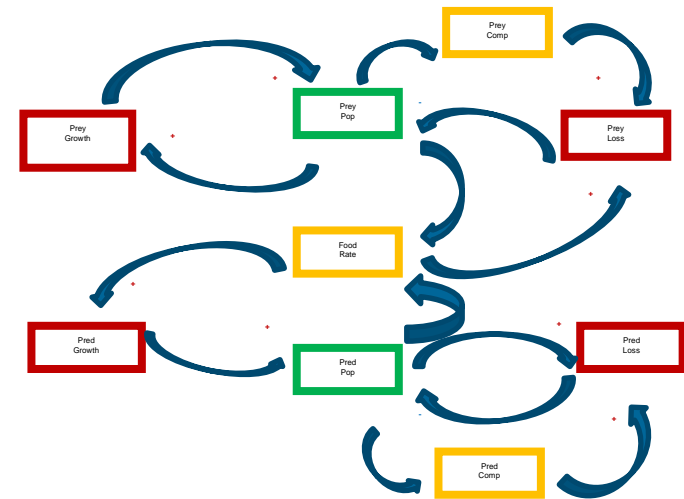
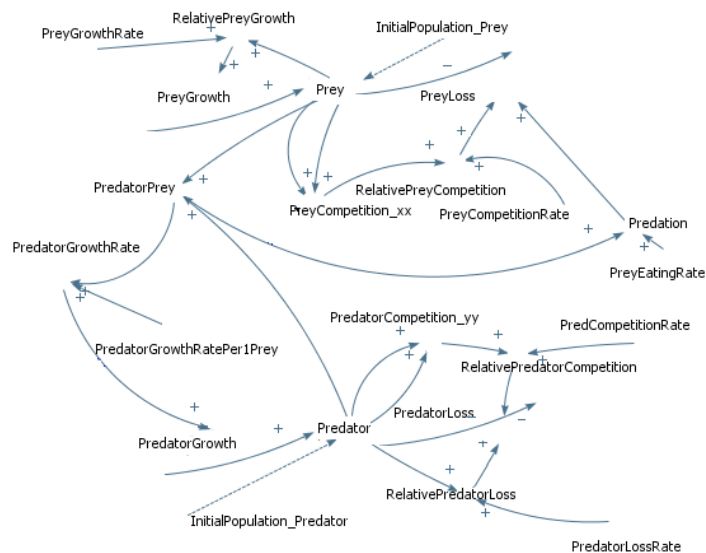
Simulation Results

Validation: Comparison & Fit of Simulation / Reality

Bad Fit

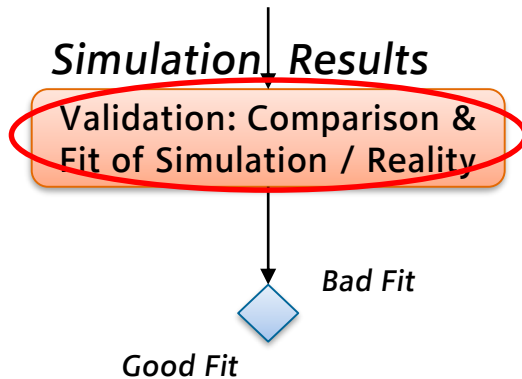
Good Fit

Causal Loop Diagram

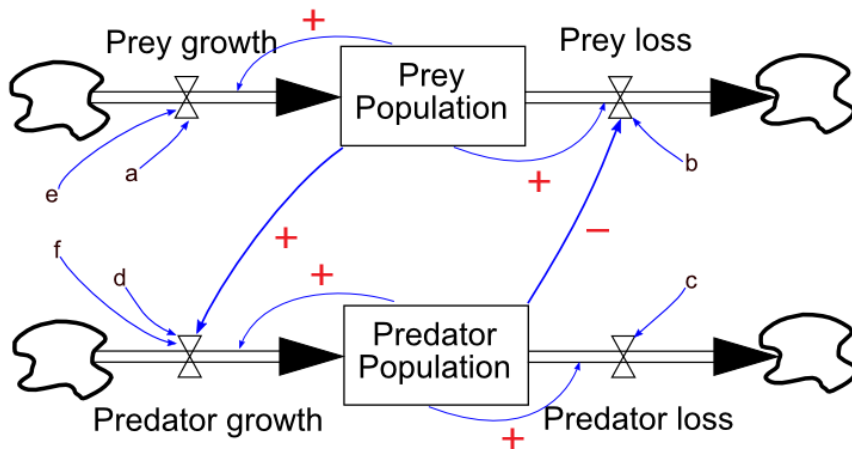
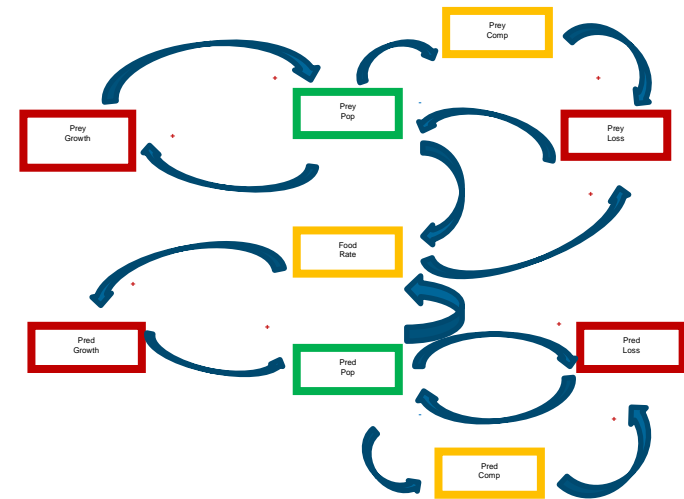


Model Extension:

- Competition Feedback



Causal Loop Diagram



Stock and Flow Diagram

Model Modification

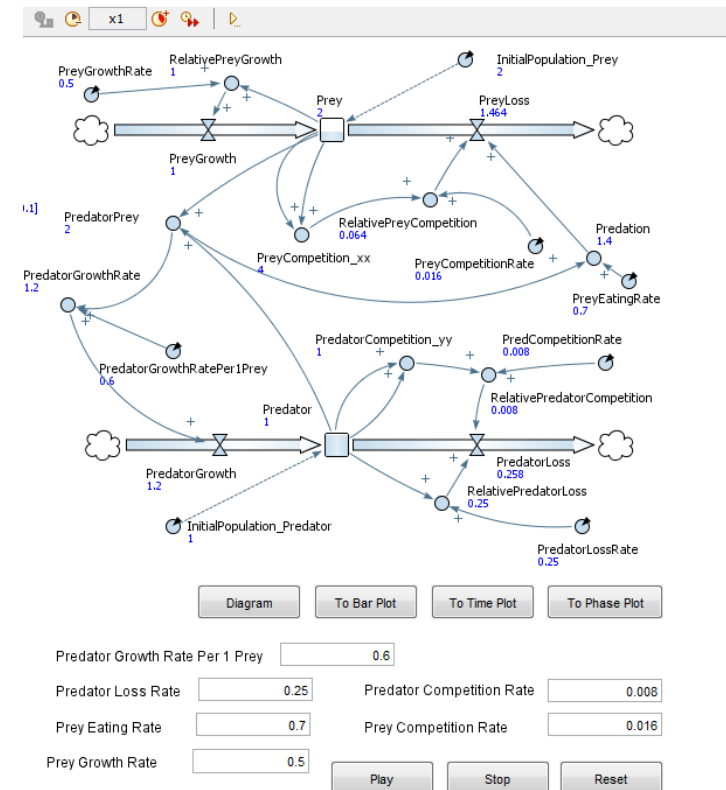
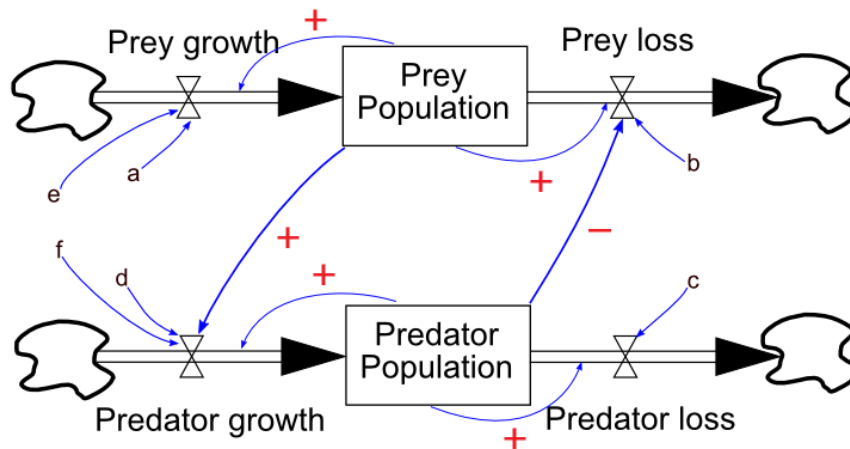
Simulation Results

Validation: Comparison & Fit of Simulation / Reality

Bad Fit

Good Fit

Stock and Flow Diagram

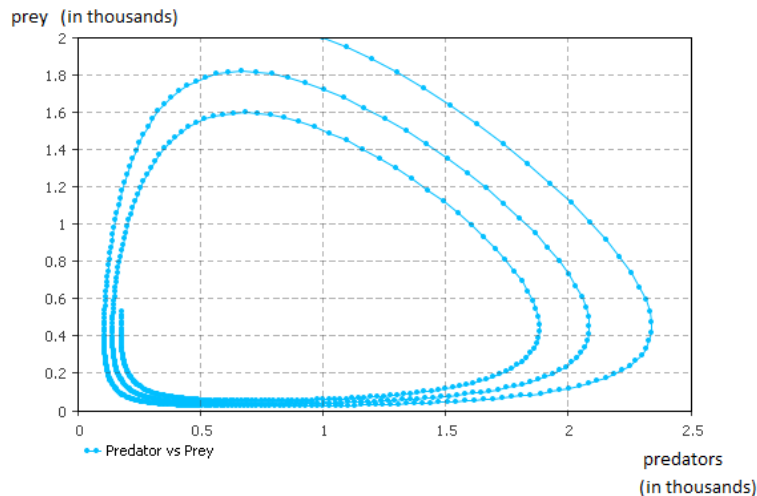


Simulation Results

Validation: Comparison & Fit of Simulation / Reality

Bad Fit

Good Fit



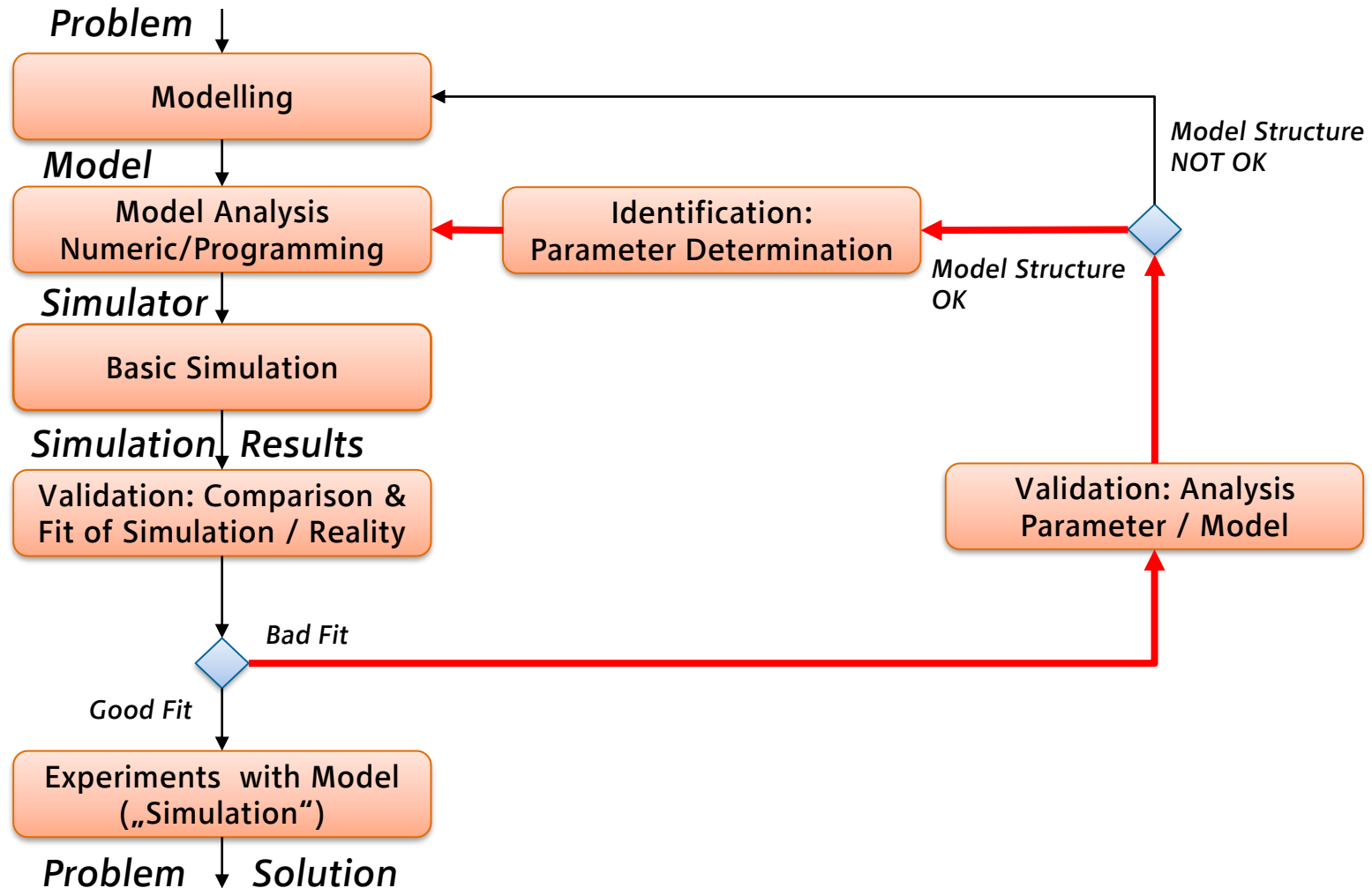
Parameters:

Predator Growth Rate Per 1 Prey	0.6
Predator Loss Rate	0.25
Prey Eating Rate	0.7
Prey Growth Rate	0.5
Predator Competition Rate	0.0080
Prey Competition Rate	0.016

$$\dot{x} = (a - b \cdot y)x - e \cdot x^2 = (a - e \cdot x - b \cdot y)x$$

$$\dot{y} = (-c + d \cdot x)y - f \cdot y^2 = (-c - f \cdot y + d \cdot x)y$$

Simulation Circle: Predator - Prey

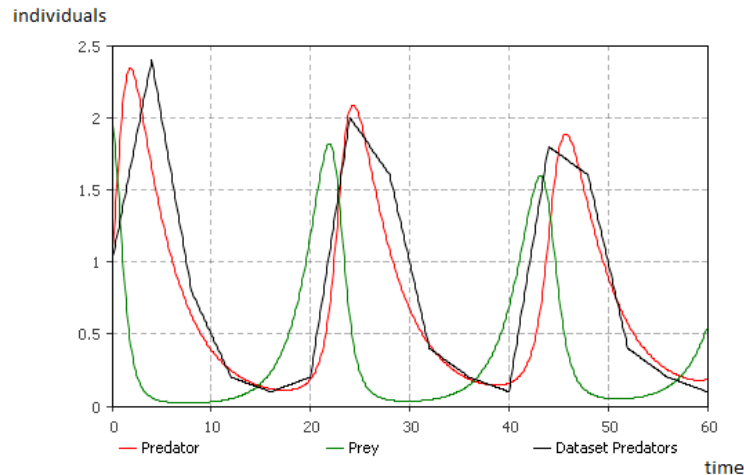


Simulation Results

Validation: Comparison & Fit of Simulation / Reality

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Good Fit



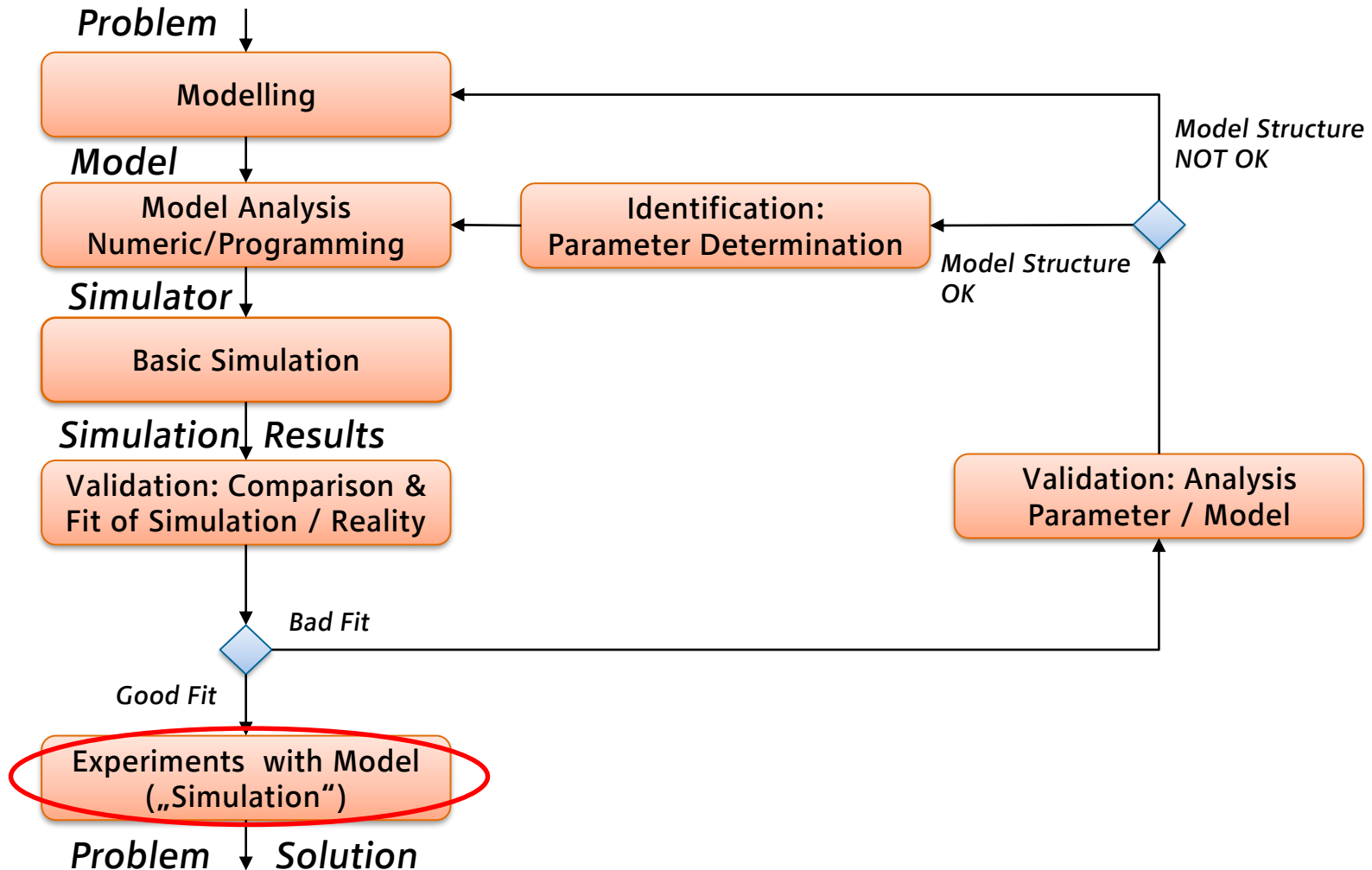
Parameters:

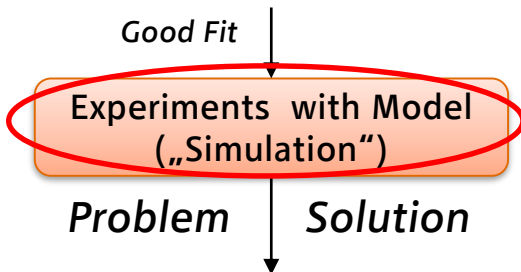
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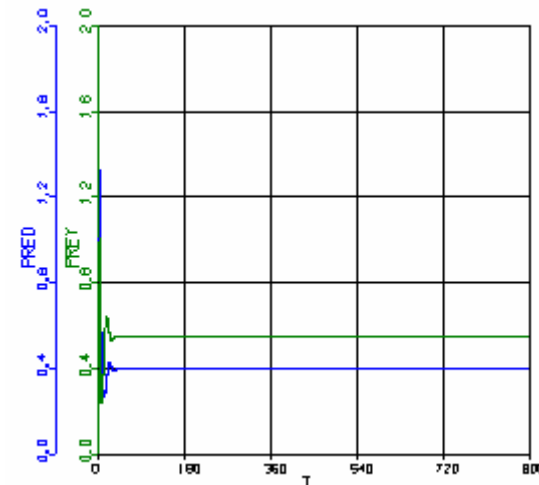
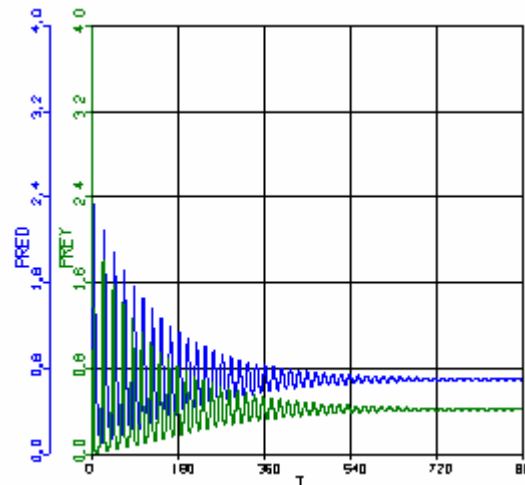
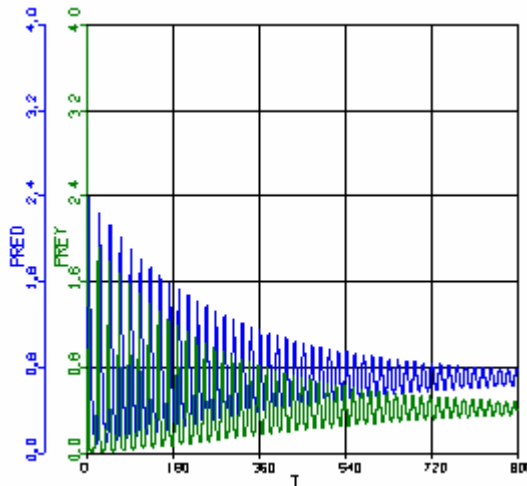
$$\dot{y} = (-c + d \cdot x)y - f \cdot y^2 = (-c - f \cdot y + d \cdot x)y$$

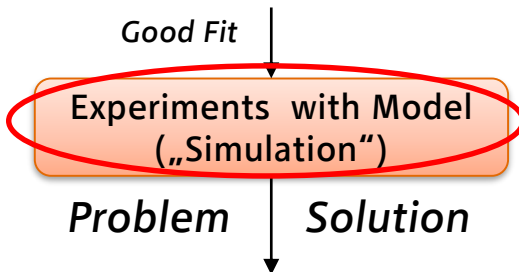
Simulation Circle: Predator - Prey



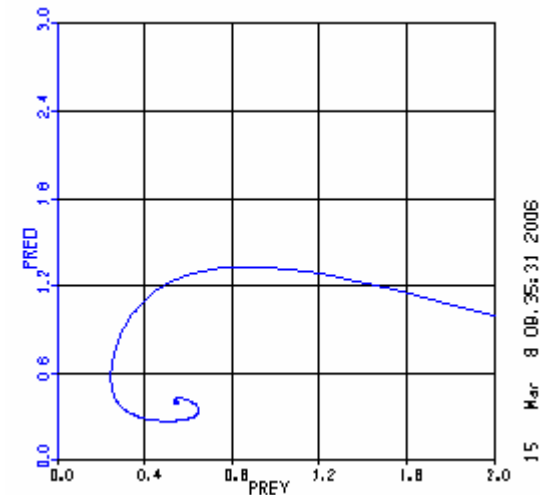
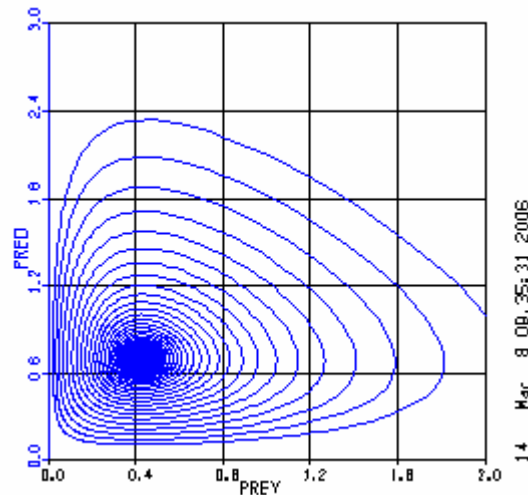
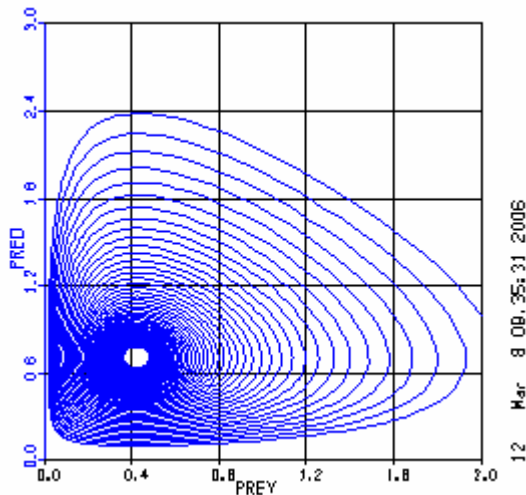


- Determination of long time behavior / stationary solutions (equilibria)



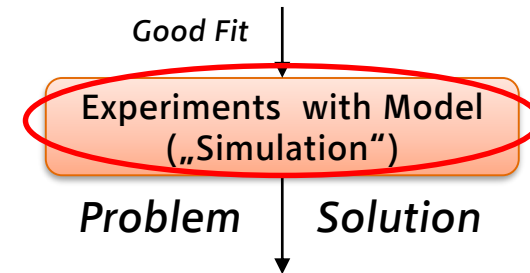


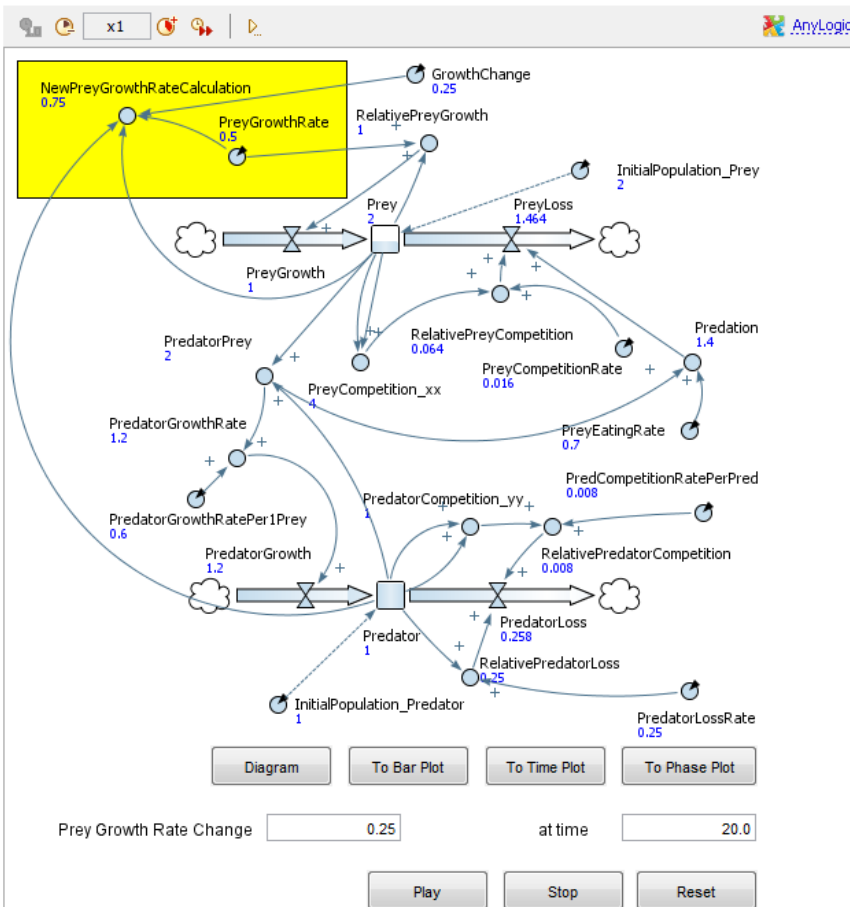
- Determination of long time behavior / stationary solutions (equilibria)



Modification of Predator-prey model with intraspecific competition

- Assume, that at a specific time poison is released into the system, e.g. some of predators are removed from the population by hunting.
- The **growth rate** a of prey is changed to:
where K is **growth rate change**.
- This change occurs at the specific time point.
- The new **growth rate** a depends on the difference between populations at this specific time point and stays constant after that.





Adequate
time instant

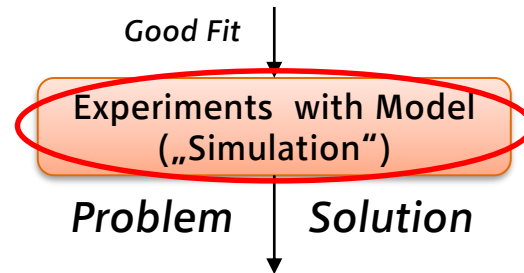
$$t_c : d_{old} \rightarrow d_{new}, \quad f_{old} \rightarrow f_{new}$$

$$\dot{x} = ax - bxy - ex^2$$

$$\dot{y} = -cy + dxy - fy^2$$

$$d_{neu} = d_{alt} + d_c (x(t_c) - y(t_c))$$

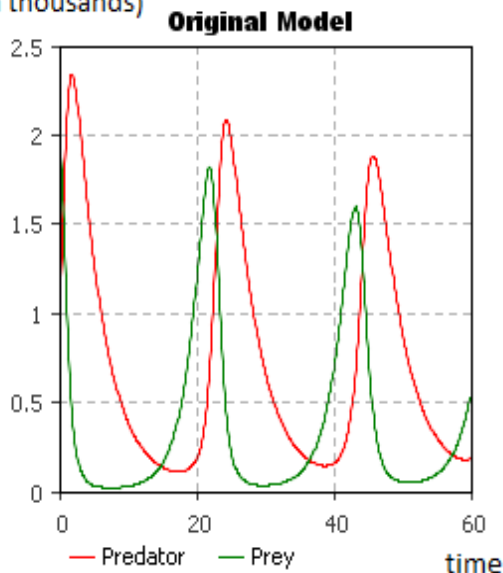
$$f_{neu} = f_c f_{alt}$$



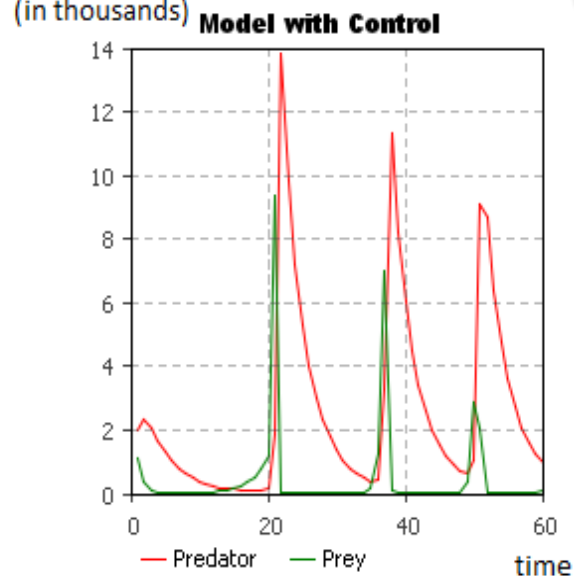
Modification of Predator-prey model with intraspecific competition

Population development over time:

individuals
(in thousands)



individuals
(in thousands)



Note: Please note the different scaling of the plots.

Good Fit

Experiments with Model
(„Simulation“)

Problem

Solution

Parameters:

Pred Loss Rate Change

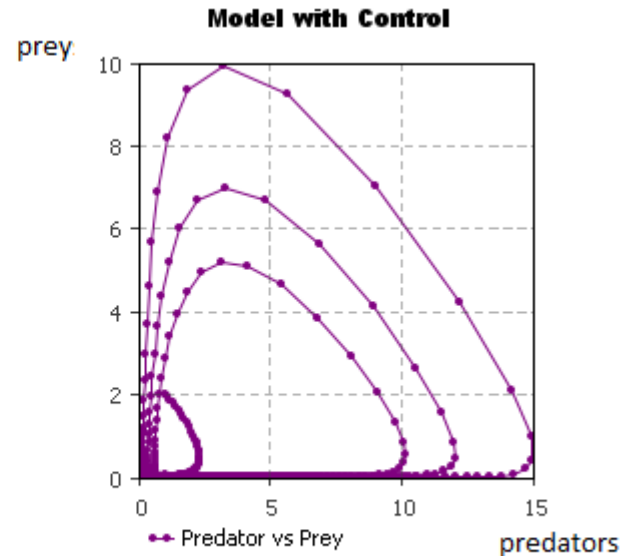
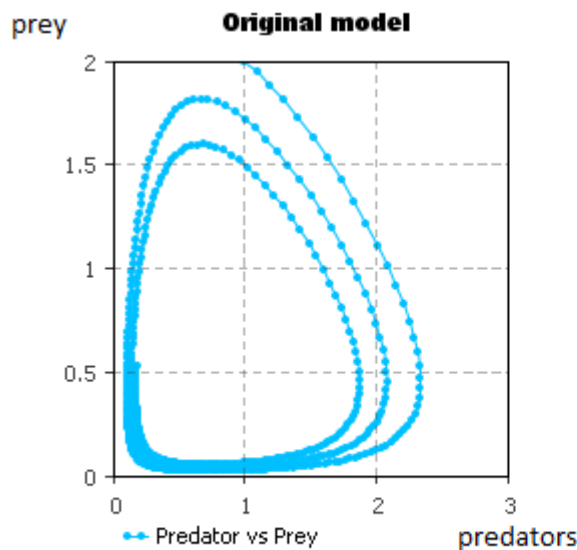
at time

$$d_{neu} = d_{alt} + d_c (x(t_c) - y(t_c))$$

$$f_{neu} = f_c f_{alt}$$

Modification of Predator-prey model with intraspecific competition

Population development over time:



Good Fit

Experiments with Model
(„Simulation“)

Problem

Solution

Parameters:

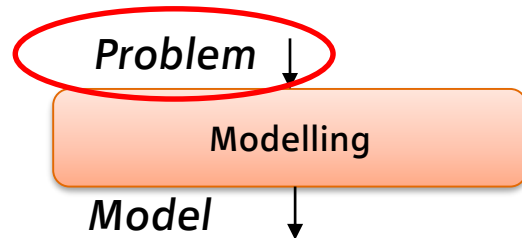
Pred Loss Rate Change

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Modification of Predator-prey model with intraspecific competition

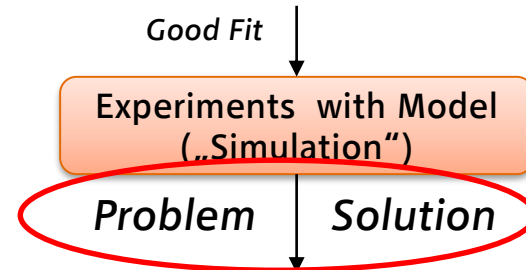


Dynamics: Prey – Predators

Environment: isolated

Measurement: natural enemies
5 Years = 60 months
quarterly

Problem: When is a reasonable time to use chemical pesticides?



Assignment: short time, changes the growth of preys, damping parameter

Approach: optimal time point t_c is dependent on the population difference

Result: The assignment is not conducive

(S. W. Golomb, Simulation 14 (1970), 197-198)

- DON'T believe that the model is the reality
- DON'T extrapolate beyond the region of fit
- DON'T distort reality to fit the model
- DON'T retain a discredited model
- DON'T fall in love with your model