

# *In Silico* Studies

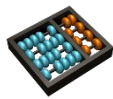
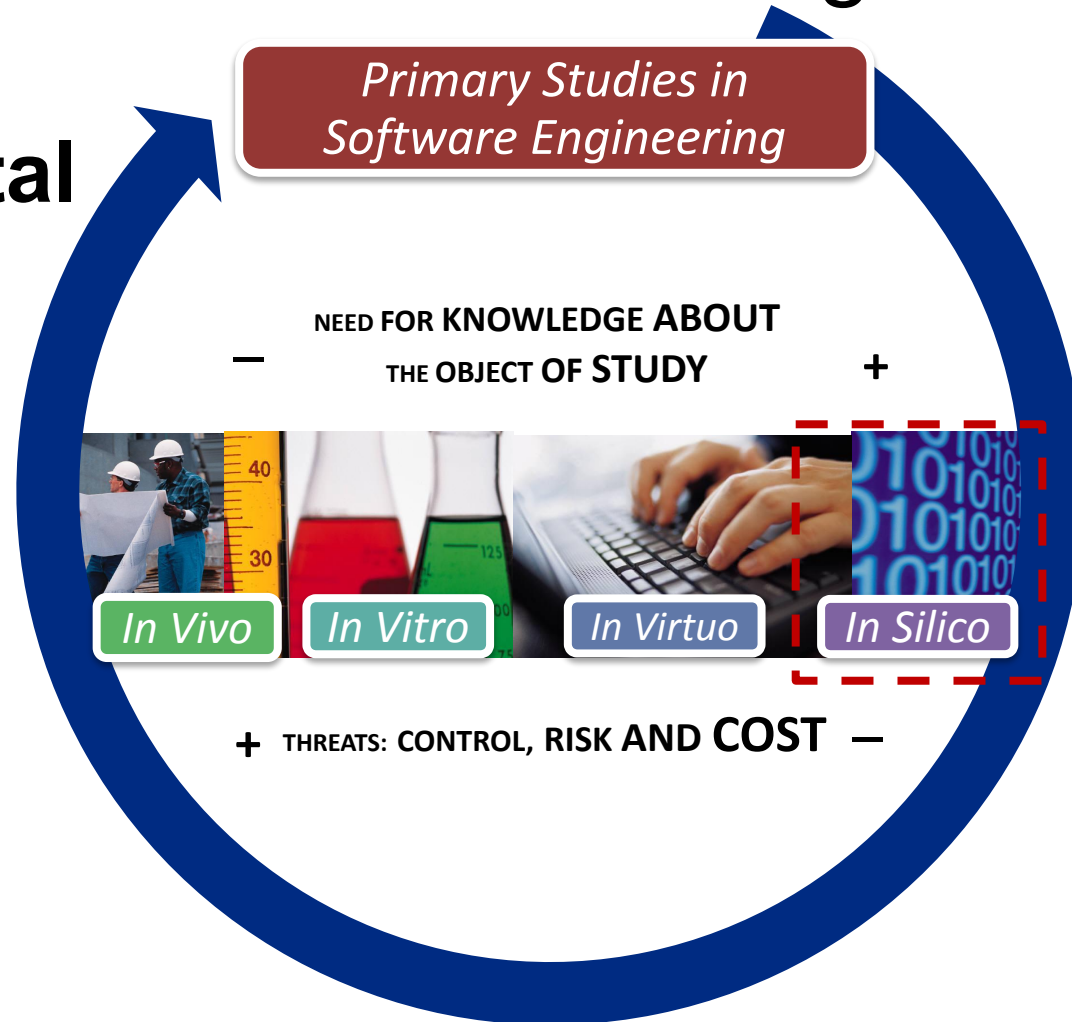
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# Environments in Software Engineering

## Experimental Cycle

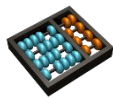
**Paradox:**  
Knowledge X Control



# Introduction

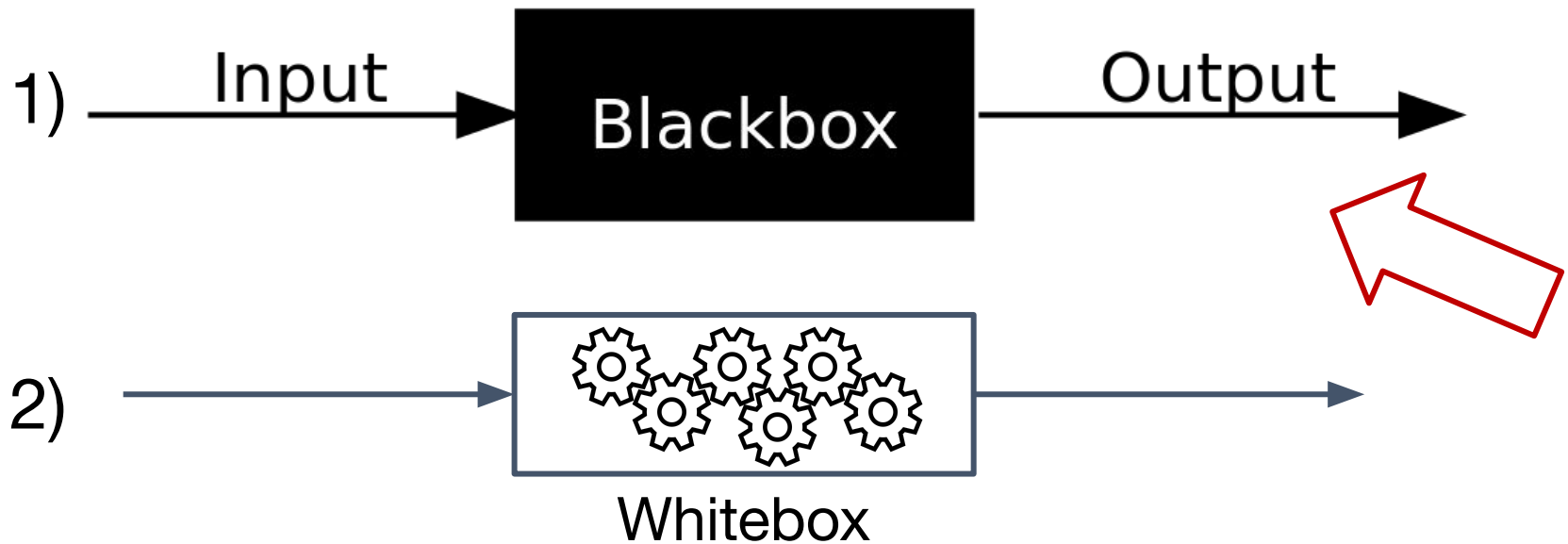
As *In Silico* studies involve the use of **computational models**, what count as a model?

- Abstractions formal enough to be understood by a computer
  - Simulation models
  - Programmed algorithms
  - State Machines
  - AI/ML models
  - ...



# Introduction

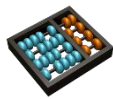
Models can be viewed in two different ways:



# Motivation for *In Silico* Studies

Conducting field or laboratory experiments can be:

- **Costly**: predicting the performance of a hardware update for all nodes in a network
- **Dangerous**: exploring alternative strategies to control a nuclear reactor
- **Last long**: assess the ecological impact of a long hunting season, for consecutive years, on the population of the species involved in a specific geographic region
- **Disturbing**: assessing the efficiency of a one-way street network within the center of an urban area
- **Morally/ethically unacceptable**: assessing the radiation dispersion of a catastrophic failure
- **Irreversible**: investigating the impact of a change in fiscal policy on a country's economy



# Advantages and Disadvantages

## Advantages of *in silico* experiments

- Make observations with high control of the environment
- Test scenarios
- Build theories
- Low time and risk
  - Enables execution of all possible combinations between the variables under investigation
- Replicate experiments



# Advantages and Disadvantages

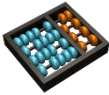
We can fail!



Credit: <https://www.goodfon.com/games/wallpaper-avariya-gonki-ogon-death.html>



Credit: <https://www.deviantart.com/puval/art/Oceanic-Flight-815-v2-80064882>



# Advantages and Disadvantages

## Disadvantages

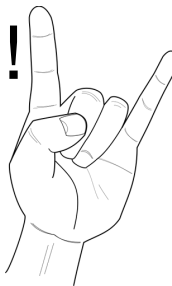
- High cost / model development effort
  - Tradeoff: develop 1 model for 1 study?
- Real-world simplifications
  - Abstraction/modeling process
  - Toy models
- How to prove model validity?



# Introduction

*How can we **experiment** with black box models?*

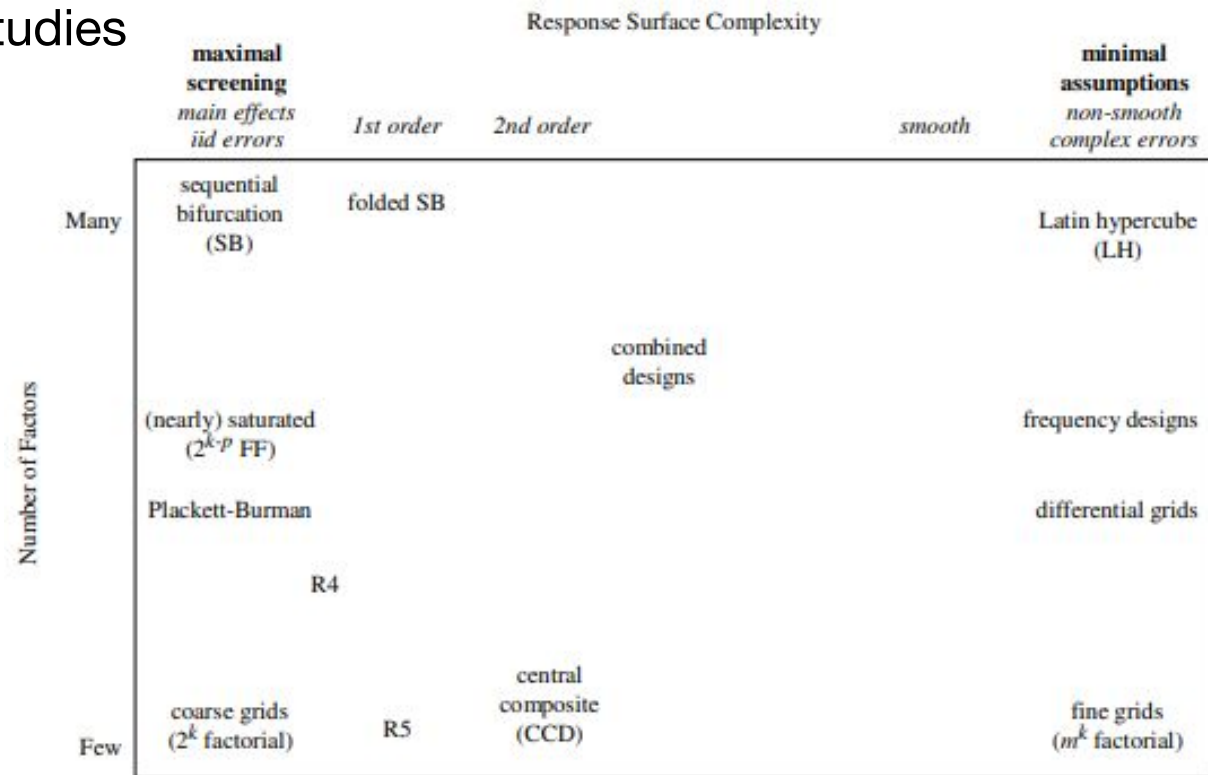
- Varying inputs
- Observing effects on the outputs
- Analyzing outputs against reference behaviors
- But, .... *How can we provoke such variation?*
  - Freely?
  - With an **experimental design**! Hell yeah!



# Experimenting with Models

## Exploration of response surface

- Multiple factors (parameters)
- Sensitivity Analysis
- Design for *in silico* (computational) studies



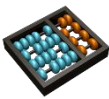
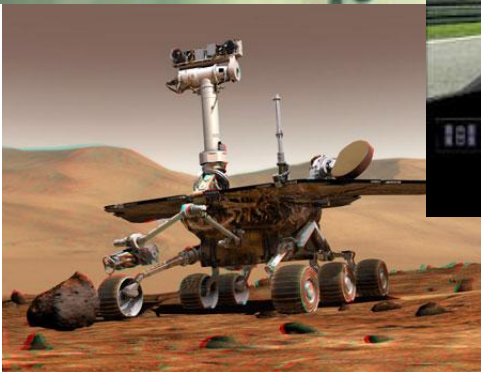
Kleijnen, J.P., Sanchez, S.M., Lucas, T.W. and Cioppa, T.M., 2005. State-of-the-art review: a user's guide to the brave new world of designing simulation experiments. *INFORMS Journal on Computing*, 17(3), pp.263-289.





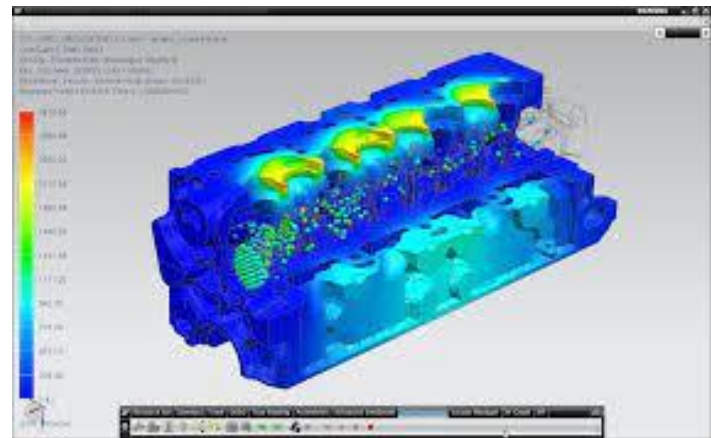
# Simulation

*When you heard the word “simulation”, what is the first thing that comes into your mind?*



# Simulation

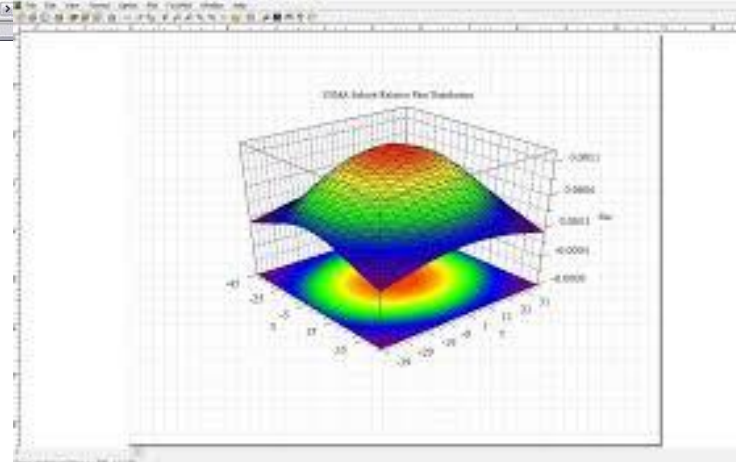
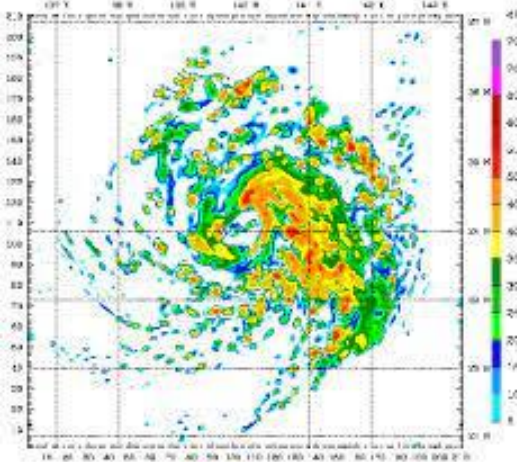
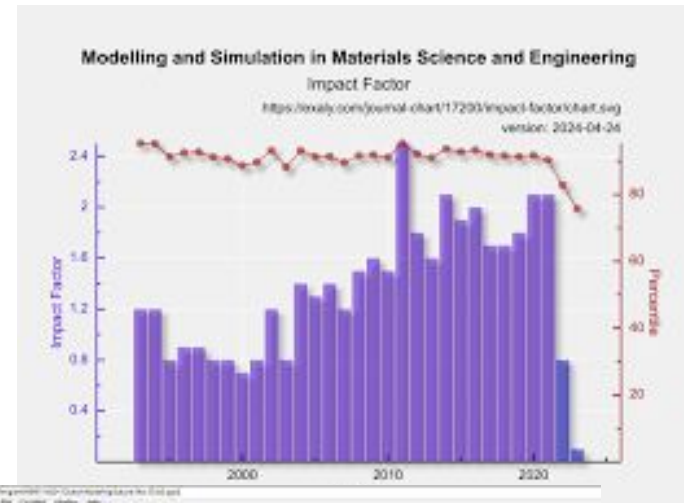
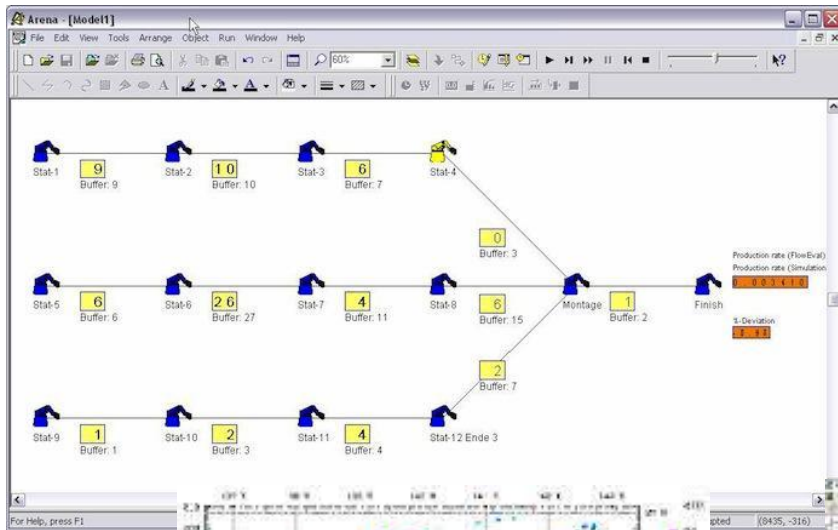
*More real applications...*





# Simulation

It's not always that fun!



# Simulation

*What is simulation?*

*“it is the imitation of a real-world process or system behavior over time. Simulation involves the generation of an artificial history of the system behavior, and the observation of such history to make inferences considering its operational characteristics”*

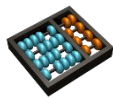
[Banks, 1999]



# Simulation

## Which systems can be simulated?

- The term “**system**” includes notions of a process or phenomenon
- The physical existence of the system is not mandatory
  - Concept, idea or proposal
- But, the system should have its “behavior as a function of time”, that is, it must be **dynamic**
  - Collection of entities interacting and producing observable behavior over a period of time
- The model is a representation or **abstraction** of the real system
  - Solution commonly used in engineering and science





# Motivation

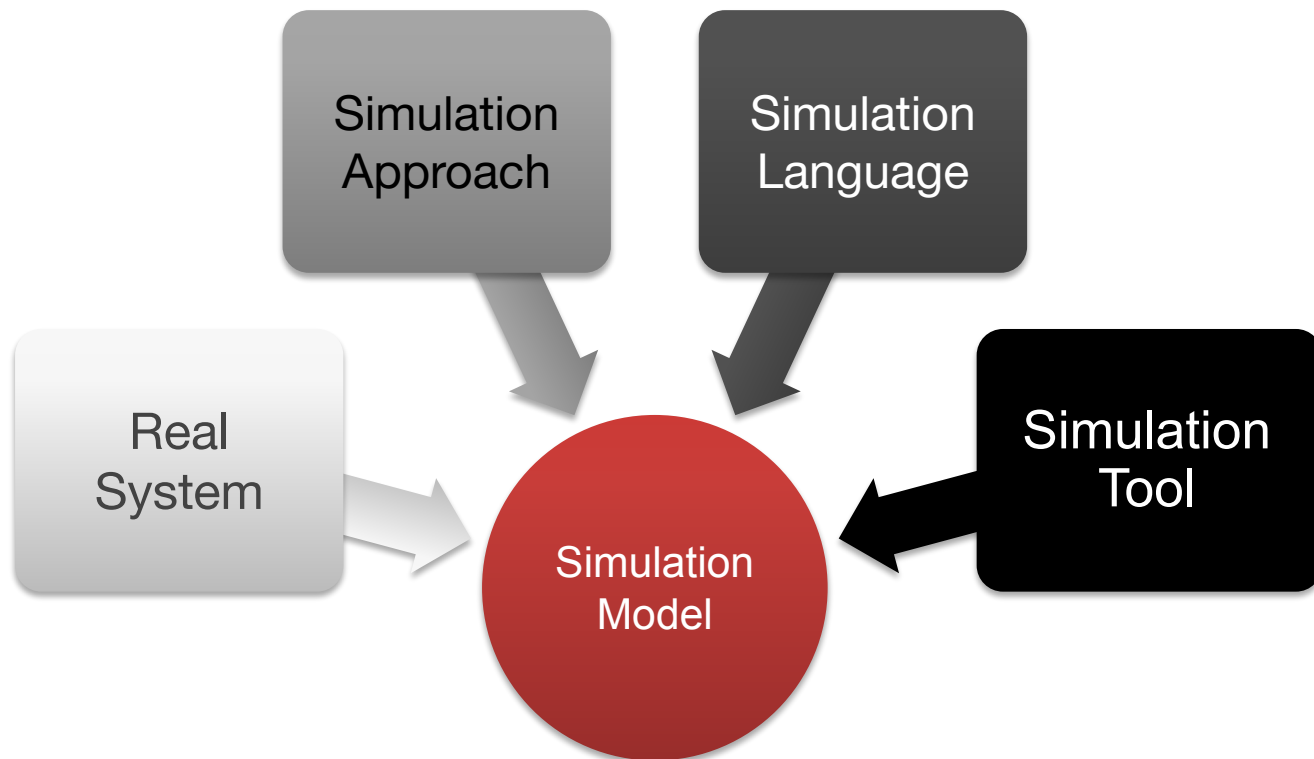
Simulation as an experimentation **instrument** in several areas of knowledge

- Biomedicine, Social Sciences, Physics and Engineering
- Automobilistic Industry
  - Crash tests
  - High-cost prototypes demanding much time/effort to build
- Pharmaceutical Industry
  - Acceleration and increase of scale for experiments
  - High-cost prototypes demanding much time/effort to build
- Opportunities to investigate problems only observed in large-scale scenarios



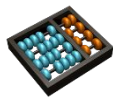
# Simulation Models

Models: mathematical formalisms, rules, graphical descriptions, or all these combined



# Simulation Elements

- **Constants and parameters:** values of characteristics or properties of the model that remain **invariant** throughout the execution of a simulation run
- **Variables:** abstraction of model characteristics whose values **vary** with the evolution of the model in the observation interval
  - **Time** is a special variable common to dynamic models
  - **Input:** external entities that represent the impact of the environment
  - **State:** define the dynamic behavior of the system
  - **Output:** characteristics of the system's behavior that motivated the model design



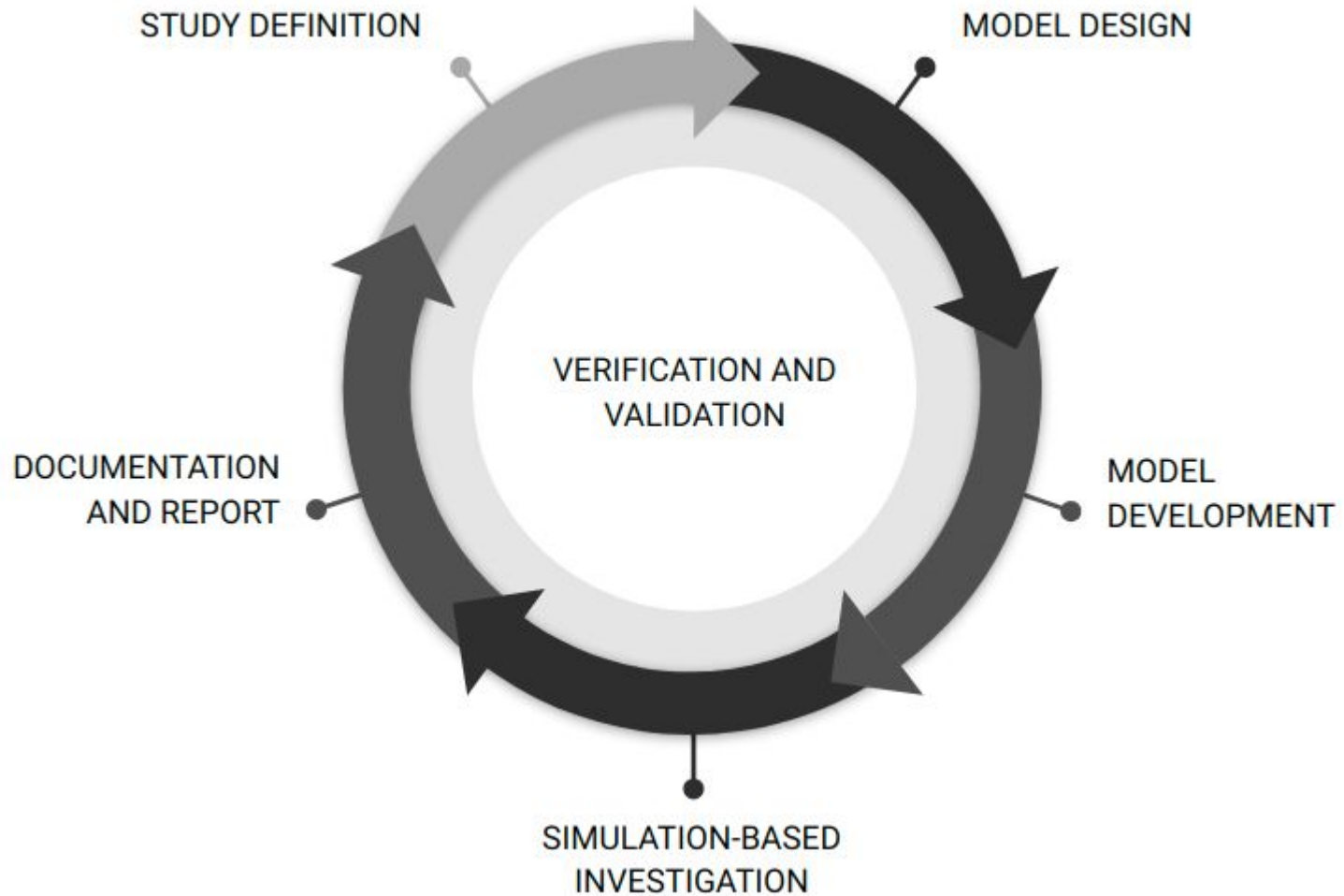
# Simulation Models Life Cycle

**Simulation-Based Studies:** “a series of steps, such as: data collection, model coding, verification and validation, experimental design, analysis of output data, and implementation”

[Alexopoulos, 2007]

Simulation models used as an **instrument** for observing the phenomenon under study

# Simulation Models Life Cycle

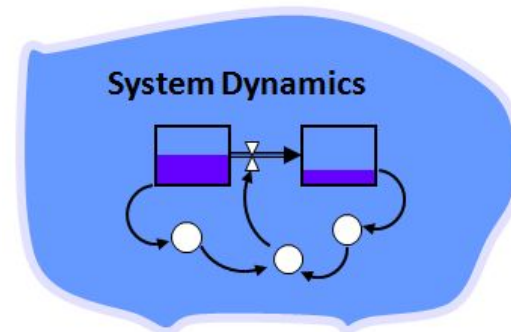
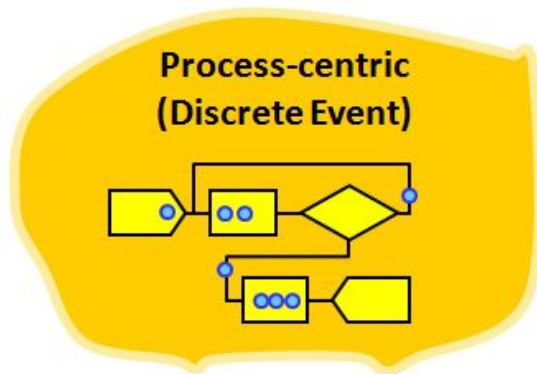


# Simulation Approaches

- Represent an abstraction
- Mechanism of advancing time
  - Simulation clock
- Determinism
- Mathematical Formalism

# Simulation Approaches

- **System Dynamics (Continuous Simulation)**
- **Discrete-Event Simulation**
- Agent-Based Simulation
- State-Based Simulation
- Hybrid Models
- ...



# System Dynamics

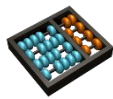
## (Continuous Simulation)

- Mathematical models for continuous systems are defined using differential equations
  - The input is specified for all values in time
- The input drives the system!

$$\frac{d}{dt} \mathbf{x}(t) = \mathbf{f}(\mathbf{x}, \mathbf{p})$$

State Variables (*stock vectors*)

Inputs (list of parâmetros)



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# System Dynamics

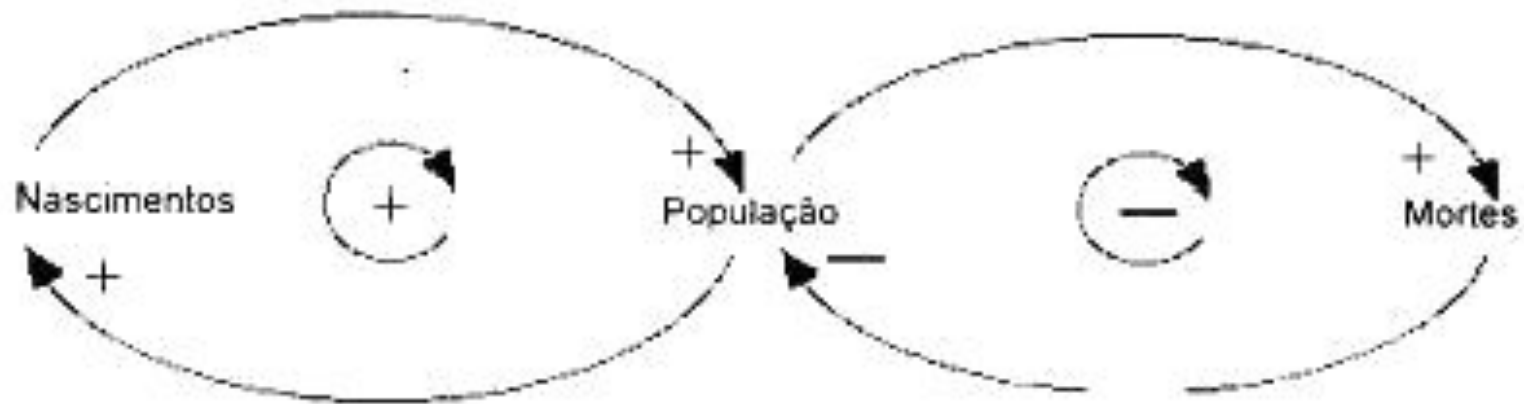
## (Continuous Simulation)

- Time advances in constant intervals
- Modelling using SD:
  - *Causal loop diagram*
    - Describes cause-effect relationships between variables
    - Positive (+) or negative (-) signs at the end of each arrow indicate how dependent variables change based on a change in an independent variable
    - Greater positive (reinforcement) and negative (balance) signals within the cycles indicate the general type of the cycle

# System Dynamics

## (Continuous Simulation)

Ex.:



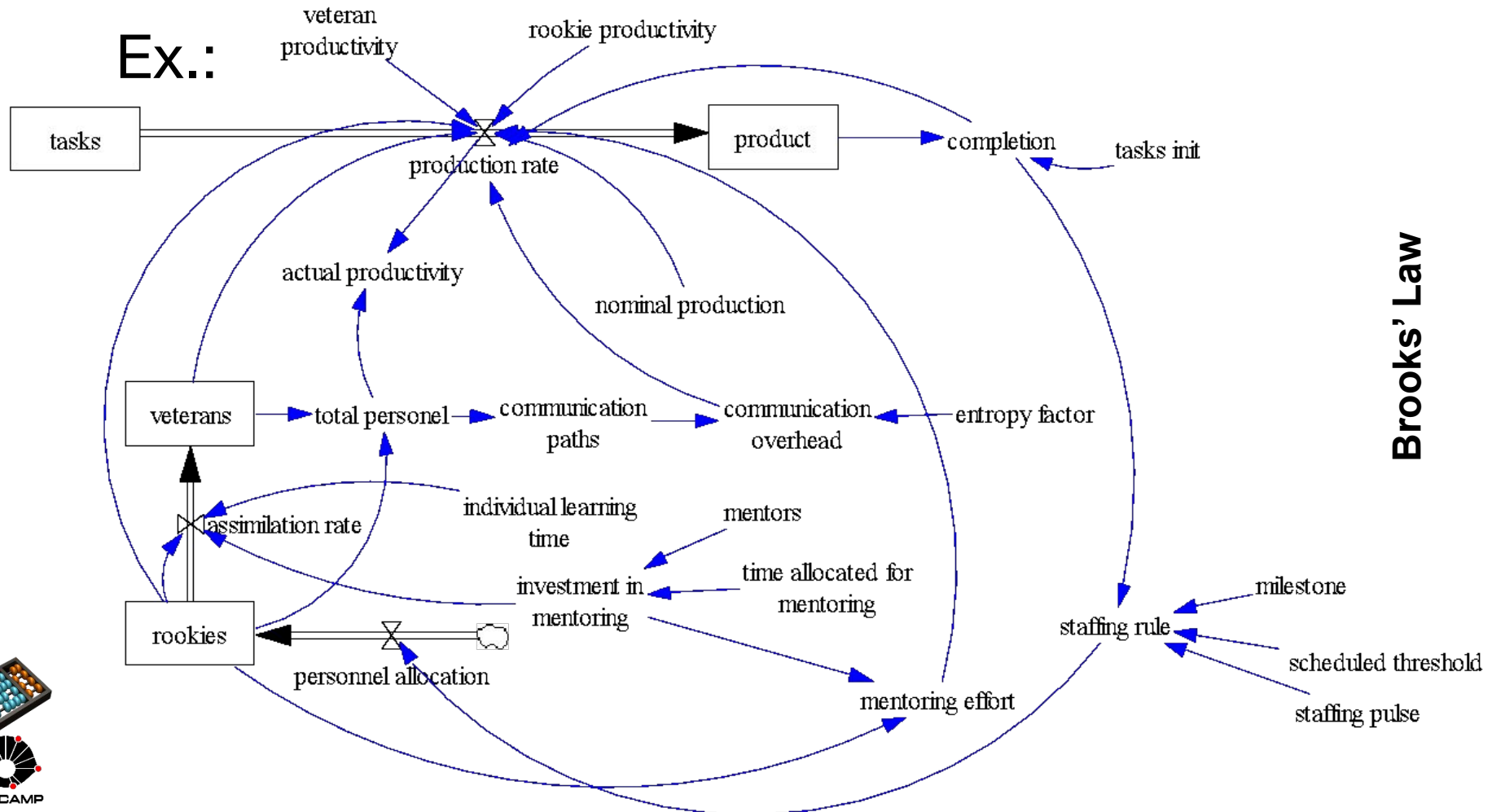
# System Dynamics

## (Continuous Simulation)

- Cause-Effect Diagram does not allow accumulation of values in variables
- Inventory (stock) and flows (rate) models
  - **Stocks:** accumulation points within the system that allow measuring the **quantity** of a variable at a given time
  - **Flows:** inventory inflows and outflows that represent the **rate** of change in inventory



# System Dynamics (Continuous Simulation)



# Discrete-Event Simulation

- Simplified view of systems based on continuous time, where
  - time  $t$  is a function of an initial time  $t_0$ , an interval  $h$ , and a discrete step  $k$
  - $t = t_0 + hk$
- Unlike continuous models, the difference is not constant, it usually varies and is non-deterministic
  - Based on stochastic methods

# Discrete-Event Simulation

- **Pseudo-random** events controlled by a list, containing the next instant that an event occurs
- Fired at  $t_0, t_1, t_2, \dots$  and are **enqueued** in such a way the system induces a pause before each message is processed
- The **processing or service** time is statistically distributed so that its duration is random, but its statistics are known

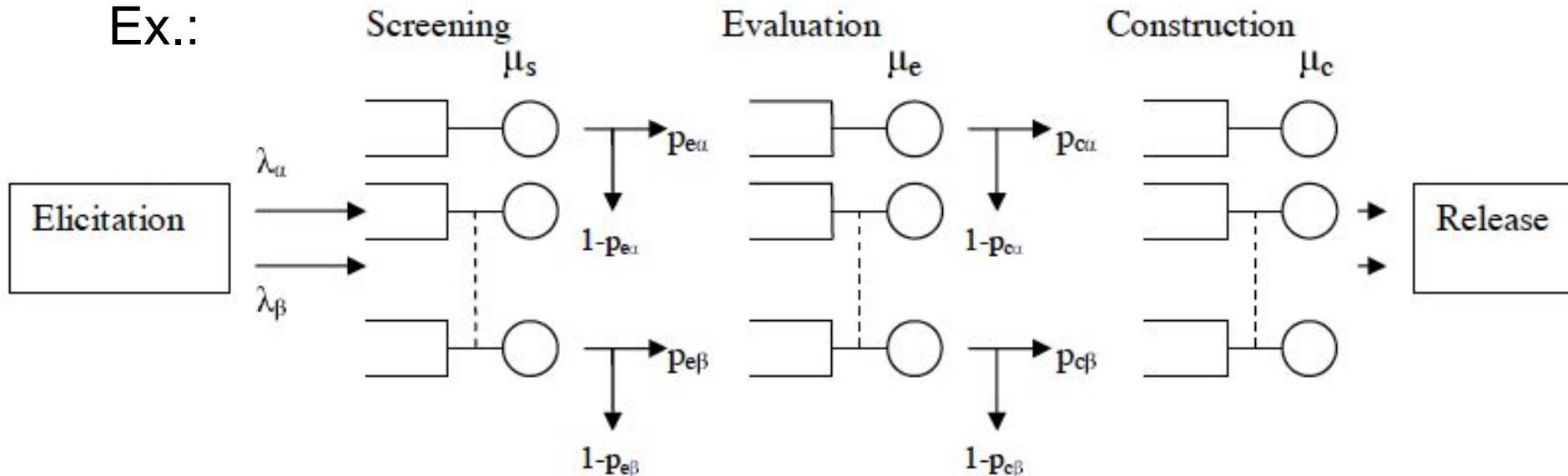


# Discrete-Event Simulation



[Höst et al, 2008]

Ex.:



# Simulation in Software Engineering

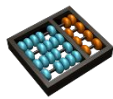
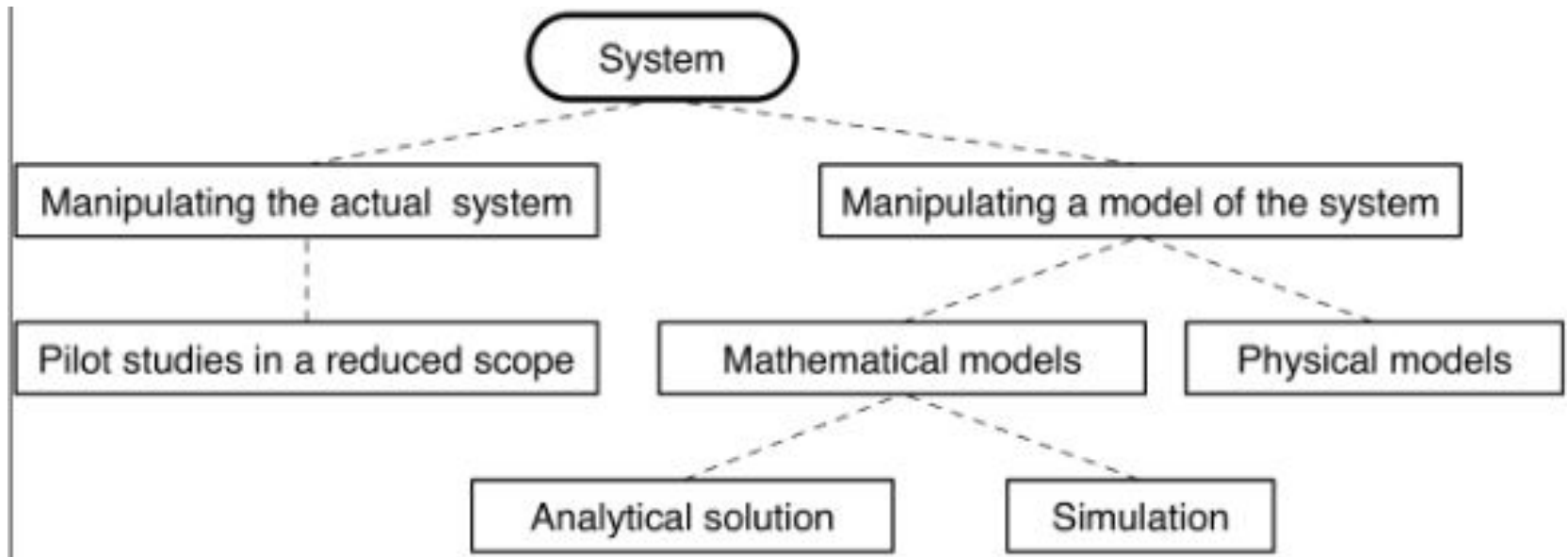


# Motivation

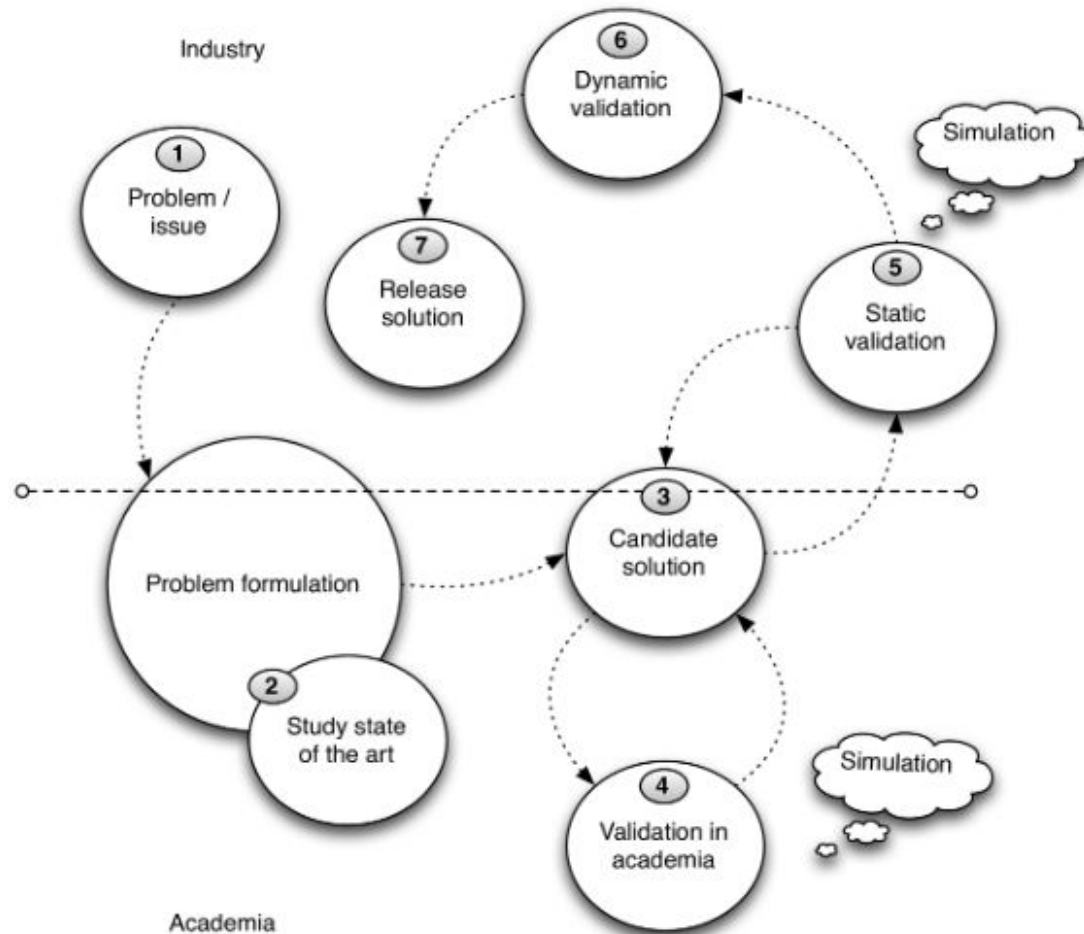
## Experimentation in Software Engineering

- Low **number of participants** in experiments
  - Reduced observation capacity (population variability)
  - Reduced generalization capacity
- **Context variables** are hard to control or even unknown
- Risks of failure during software systems or projects execution, or during the phenomenon observation

# Motivation



# Simulation in Software Engineering



# Secondary Studies on Simulation in SE

## SLR: Software process simulation from 1998 to 2008

- ~ 200 studies [Zhang et al, 2008]
- Findings:
  - **Classification** of software process simulation models;
  - Improvement for models **efficiency**;
  - **Hybrid models** provide more realistic models.

## SMS: Simulation in SE until 2011

- 108 studies [de França and Travassos, 2013]
- Findings:
  - Concentration on software process and project;
  - System Dynamics and DEVS
  - Lack of research agenda and rigor
  - Poor-quality reports
  - Need for methodological support

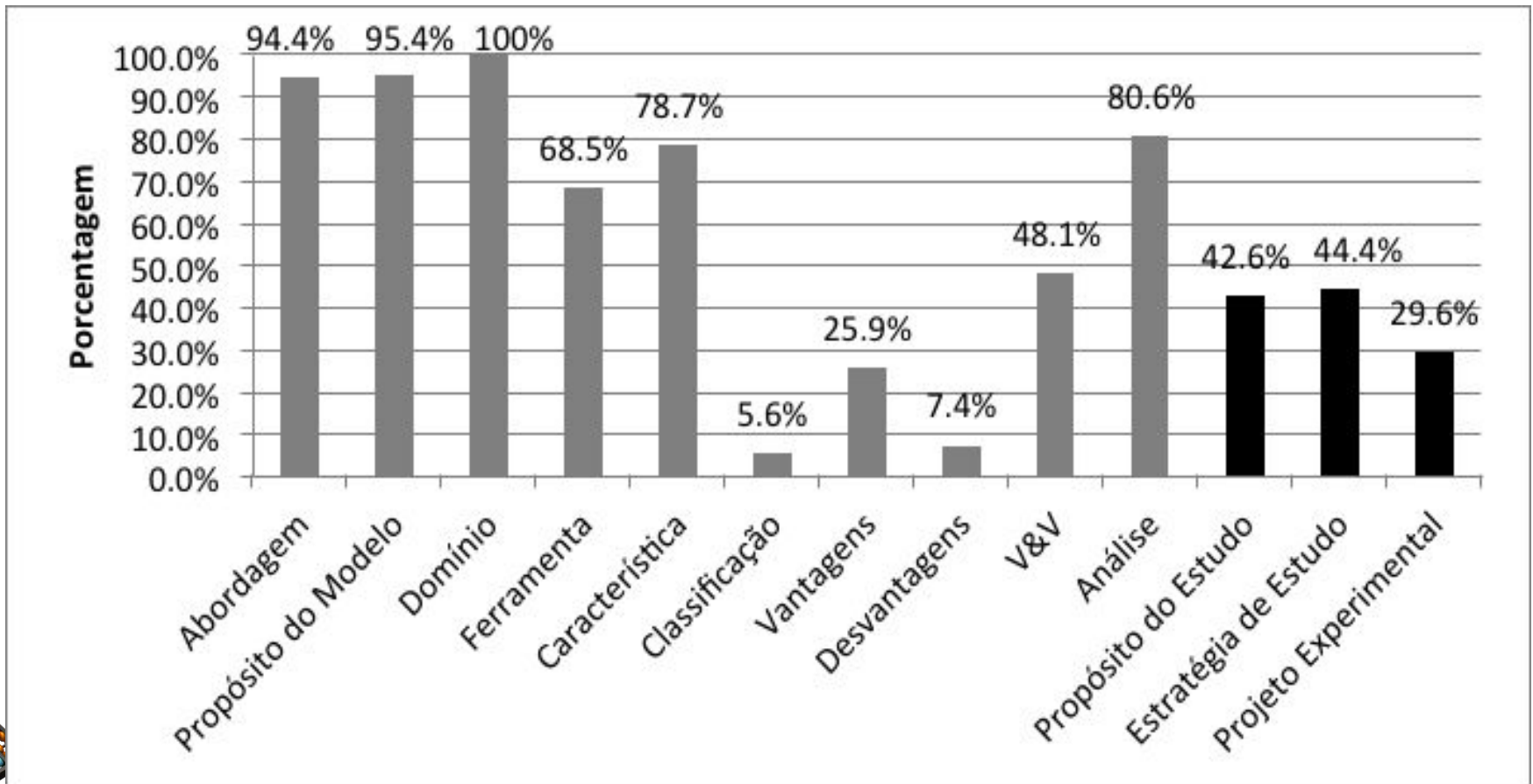


# Secondary Studies on Simulation in SE

SMS: software process simulation in industry until 2013

- 87 studies [Ali, Petersen and Wohlin, 2014]
- Findings:
  - Proof-of-concepts with different purposes (estimation, training, process improvement, etc.)
  - Low-quality studies
  - Models are insufficiently validated regarding their purpose
  - Lack of evidence regarding the usefulness of SPS
  - According to reported costs, one cannot say it is a low-cost method
  - Need for methodological support on conducting and reporting SBS

# Report Quality



de França, B.B.N.; Travassos, G.H. Are We Prepared for Simulation Based Studies in Software Engineering yet? CLEI eletronic journal, CLEIej, v. 16, n. 1, paper 8, April, 2013.



# Simulation in Software Engineering

Threats to validity are different from the other methods

From Context to Research Questions

Simulation Feasibility

Simulation Model

**Model Validation**

Subjects (*in virtuo* and *in silico*)

Experimental Design

Intermediate Experimental Trials

Supporting Data

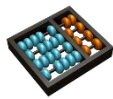
Simulation Environment

Output Analysis

Study Report

↑ Threats to Validity ↓

Avoid some risks but  
introduce new ones



# SBS Planning and Reporting Guidelines

ID	Guideline Statement
<b>Identification</b>	
<b>SG1</b>	Proper title and keywords should objectively identify the simulation study, and a structured abstract should summarize its contents
<b>From Context to Research Questions</b>	
<b>SG2</b>	The context where the simulation study is taking place should be captured in full
<b>SG3</b>	Explicitly state the problem motivating the simulation study, so that research questions can be derived
<b>SG4</b>	Clearly state the simulation study goals and scope
<b>SG5</b>	Derive the research questions from the established goals
<b>SG6</b>	Clearly state the null and alternatives hypotheses from the research questions
<b>Simulation Feasibility</b>	
<b>SG7</b>	Present justifications for considering simulation studies as the ideal or feasible observation strategy
<b>Background and related work</b>	
<b>SG8</b>	Present only essential background knowledge and the related works
<b>Simulation Model Specification</b>	
<b>SG9</b>	Have a detailed description and understanding of both conceptual and executable simulation models, as well as its variables, equations, input parameters and the underlying simulation approach
<b>Simulation Model Validation</b>	
<b>SG10</b>	Gather all evidence regarding the simulation model (conceptual and execution) validity
<b>SG11</b>	Make use of Face Validity procedure (involving domain experts) to assess the plausibility of both conceptual and executable models and simulation outcomes, using proper diagrams and statistical charts as instruments respectively



# SBS Planning and Reporting Guidelines

ID	Guideline Statement
<b>SG12</b>	Support model (causal) relationships, as much as possible, with empirical evidence to reinforce their validity and draw more reliable conclusions
<b>SG13</b>	Always verify the model assumptions, so the results of simulated experiments can get more reliable
<b>Subjects</b>	
<b>SG14</b>	Characterize the subjects involved in the simulation study as well as their training needs
<b>Experimental Design</b>	
<b>SG15</b>	Describe the experimental design (design matrix), including independent and dependent variables and how levels are assigned to each factor
<b>SG16</b>	Use Sensitivity Analysis to select valid parameters settings when running simulation experiments, rather than model “fishing”.
<b>SG17</b>	Consider as factors (and levels) not only the simulation model’s input parameters when designing the simulation experiment, but also internal parameters, different sample datasets and simulation model versions, implementing alternative strategies to be evaluated
<b>SG18</b>	When adopting ad-hoc design determine the selected simulation scenarios and explain the criteria used to identify them as relevant
<b>SG19</b>	When dealing with simulation model containing stochastic components, determine the number of runs required for each scenario, along with its rationale, in order to capture the phenomenon variance.

# SBS Planning and Reporting Guidelines

Supporting Data	
<b>SG20</b>	Assess, whenever possible, the data used to support the simulation model development or experimentation
<b>SG21</b>	Keep track of contextual information (including qualitative data) along with quantitative data
<b>SG22</b>	Make sure that both calibration and experiment datasets came from the same population
Simulation Supporting Environment	
<b>SG23</b>	Set up and describe the simulation environment, including the supporting tools, associated costs, and decision for using a specific simulation package
<b>SG24</b>	Determine which and how intermediate measures are stored among simulation trials to be used in the final analysis
Output Analysis	
<b>SG25</b>	Determine which statistical procedures and instruments support the output analysis, as well as the underlying rationale, quantifying the amount of internal variation embedded in the (stochastic) simulation model to augment the precision of results
<b>SG26</b>	Be aware about data validity when comparing actual and simulated results: compared data must come from the same or similar measurement contexts
Threats to Validity	
<b>SG27</b>	Consider to check for threats to the simulation study validity before running the experiment and analysing output data to avoid bias, as well as to report non-mitigated threats, limitations and non-verified assumptions
Conclusions and Future Works	
<b>SG28</b>	Main results/findings should be identified and summarized, as well as the conclusions arising from the results.
<b>SG29</b>	Applicability issues should be addressed in the report, considering organizational changes and associated risks.
<b>SG30</b>	Point out future research directions and challenges after current results.

# SBS Planning - Study Definition

## Context (SG2):

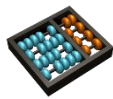
Exploration of the Brooks' Law for Software Project Management using a System Dynamics model.

*“Adding manpower to a late software project makes it later.”*



## Problem (SG3)

In the middle of the 70s, Fred Brooks stated (based on his experiences) this law as a generalized phenomenon for every software project. **However**, years later, several empirical evidence has show different contexts in which the law may need an *addendum* in order to still be considered valid. **Thus**, project managers and leaders need to be aware of the right scenarios they can overcome the effects of the Brooks' Law.

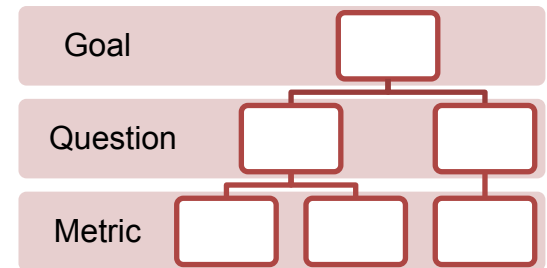




# SBS Planning - Study Definition

## Goal (SG4)

Analyze the Brooks' Law behavior/dynamics  
For the purpose of characterizing  
With respect to the need for adequacy  
From the point of view of software engineering  
researchers  
In the context of a System Dynamics model for  
simulating software project scenarios



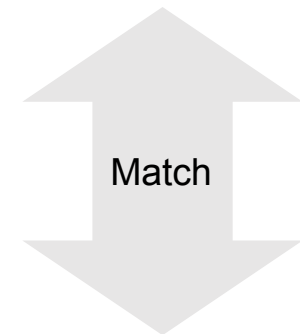
## Questions (SG5)

RQ: Does Brooks' Law need to be adapted to specific  
real-life scenarios? If yes, what are these scenarios?

## Hypotheses (SG6)

This may be optional for characterization or exploratory  
studies. If you are supposed to test some, so it is  
mandatory

Model Purpose



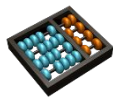
Study Goals



# SBS Planning - Study Definition

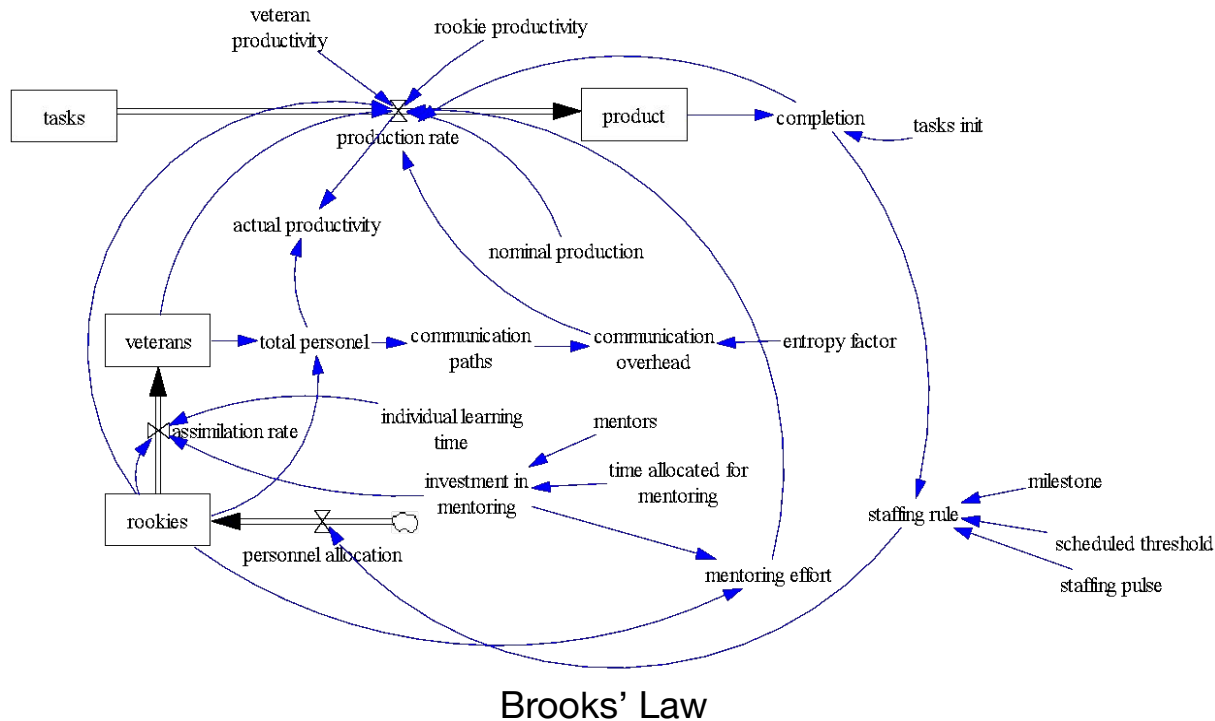
## Justification for Simulation (SG7)

- Experimenting with running software projects may be time and resource-consuming
- Experimenting with software projects in different personnel configurations is impractical
- Controlling amount of personnel is hard or unpredictable in the long run
- Making software projects later is risky and wastes resources
- ...



# SBS Planning - Model

## Simulation Model (SG9) and its Validity (SG10)



### Validity Evidence:

- Conceptual validity (SG12)
- Model testing
- Face validity (SG11)

### Model Assumptions (SG13)



# Verification and Validation

Procedure	Description
Face Validity	Consists of getting feedback from individuals knowledgeable about the phenomenon of interest through reviews, interviews, or surveys, to evaluate whether the (conceptual) simulation model and its results (input-output relationships) are reasonable.
Comparison with Reference Behaviors	Compare the simulation output results against trends or expected results often reported in the technical literature.
Comparison with Other Models	Compare the results (outputs) of the simulation model being validated to results of other valid (simulation or analytic) model. Controlled experiments can be used to arrange such comparisons.
Event Validity	Compare the “events” of occurrences of the simulation model to those of the real phenomenon to determine if they are similar. This technique is applicable for event-driven models.
Historical Data Validation	If historical data exists, part of the data is used to build the model and the remaining data are used to compare the model behavior and the actual phenomenon. Such testing is conducted by driving the simulation model with either sample from distributions or traces, and it is likely used for measuring model accuracy.
Rationalism	Use logic deductions from model assumptions to develop the correct (valid) model, by assuming that everyone knows whether the clearly stated underlying assumptions are true.

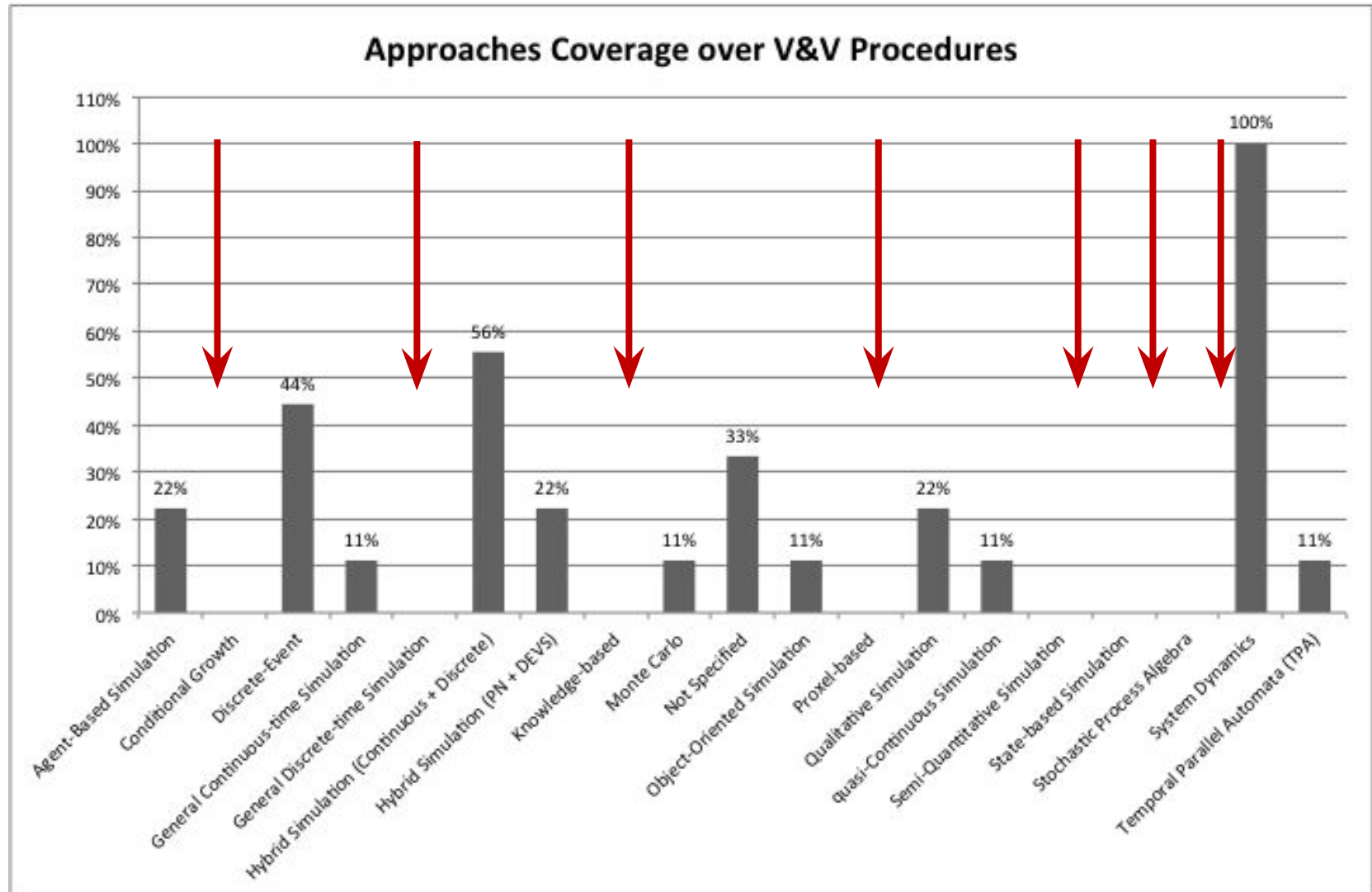
# Verification and Validation

- Predictive Validation** Use the model to forecast the phenomenon behavior, and then compares this behavior to the model forecast to determine if they are the same. The phenomenon data may come from the real phenomenon observation or be obtained by conducting experiments, e.g., field tests for provoking its occurrence. Also, data from the technical literature may be used, when there is no complete data in hands.
- Internal Validity** It is likely used for measuring model accuracy. Several runs of a stochastic model are made to determine the amount of (internal) stochastic variability. A large amount of variability (lack of consistency) may cause the model results to be questionable, even if typical of the problem under investigation.
- Sensitivity Analysis** Consists of systematically changing the values of the input and internal parameters of a model to determine the effect upon the model output. The same relationships should occur in the model as in the real phenomenon. This technique can be used qualitatively – trends only – and quantitatively – both directions and (precise) magnitudes of outputs.
- Testing model structure and behavior** Submit the simulation model to tests cases, evaluating its responses and traces. Both model structure and outputs should be reasonable for any combination of values of model inputs, including extreme and unlikely ones. Besides, the degeneracy of the model behavior can be tested by appropriate selection of values of parameters.
- Based on empirical evidence** Collect evidence from the technical literature (experimental studies reports) to develop the model causal relationships (mechanisms).
- Turing Tests** Individuals knowledgeable about the phenomenon are asked if they can distinguish between real and model outputs.





# Verification and Validation



# SBS Planning - Design

## Experimental Design (SG15 and SG18)

Possible factors: rookie and veteran productivity, nominal productivity, entropy factor, mentors, time allocated for mentoring, individual learning time, milestone, schedule threshold, and staffing pulse. I.e., all the **independent variables**. *What else (SG17)?*

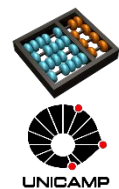
A full exploratory study would consider all these variables at different levels (SG16).

Here, let's take the **entropy factor** and the **staffing pulse** as examples.

Trial	Staffing Pulse	Entropy Factor
1	0	0.03
2	2	0.03
3	4	0.03
4	6	0.03
5	0	0.06
6	2	0.06
7	4	0.06
8	6	0.06

## Number of Runs (SG19)

8, the same number of trials/scenarios as the model is deterministic.



# SBS Planning - Environment

## Supporting Data (SG20)

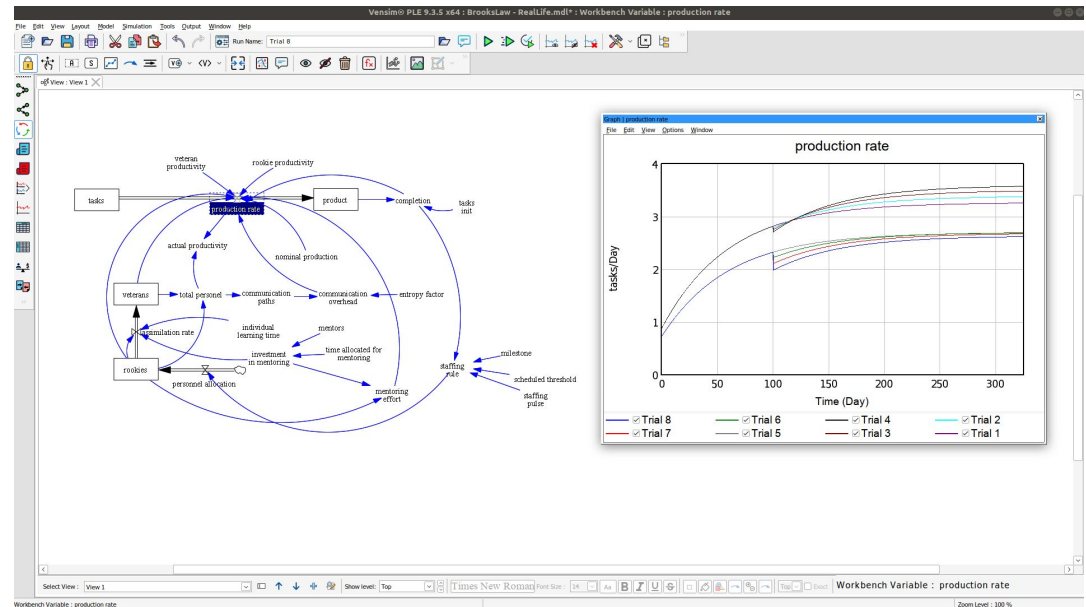
Model equations and constants were calibrated but no data is available. No additional data required. So, neither SG21 (qualitative/contextual data) and SG22 (calibration and datasets) could be applied.

## Simulation Environment (SG23)

Vensim PLE 9.3.5

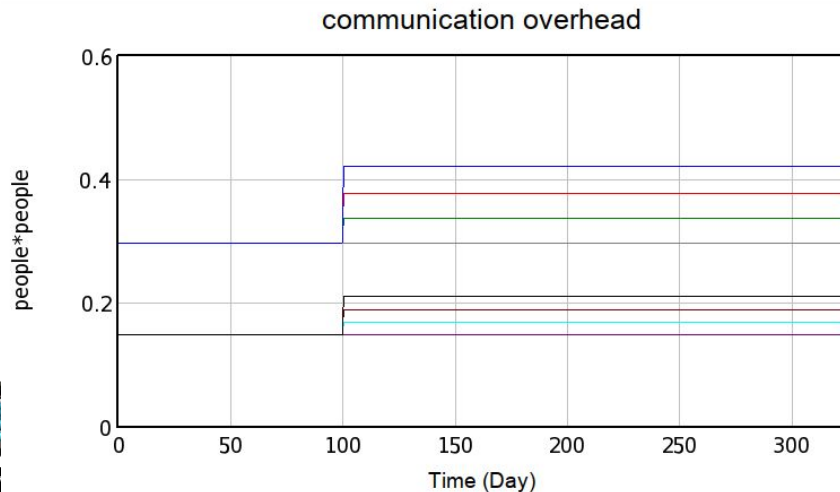
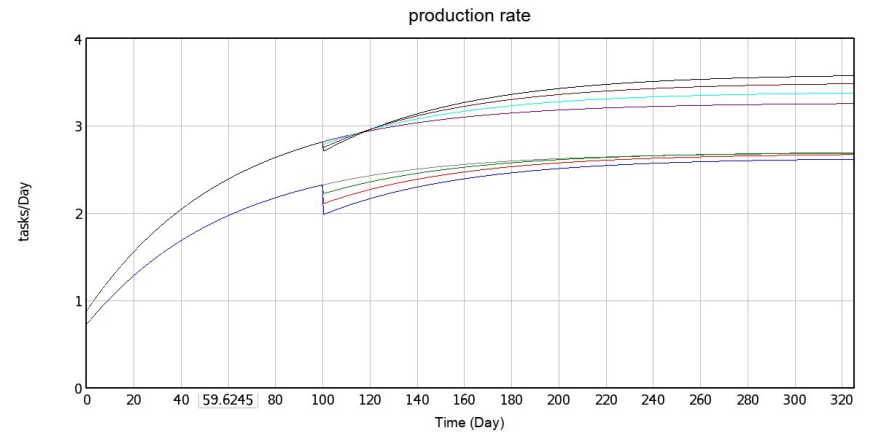
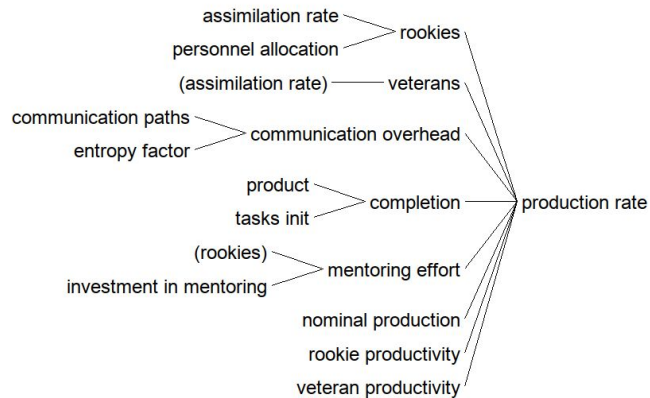
Notebook dell inspiron i7

16Gb RAM



# SBS Planning - Environment

## Output Analysis (SG25)



Legend for production rate graph:

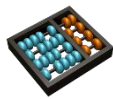
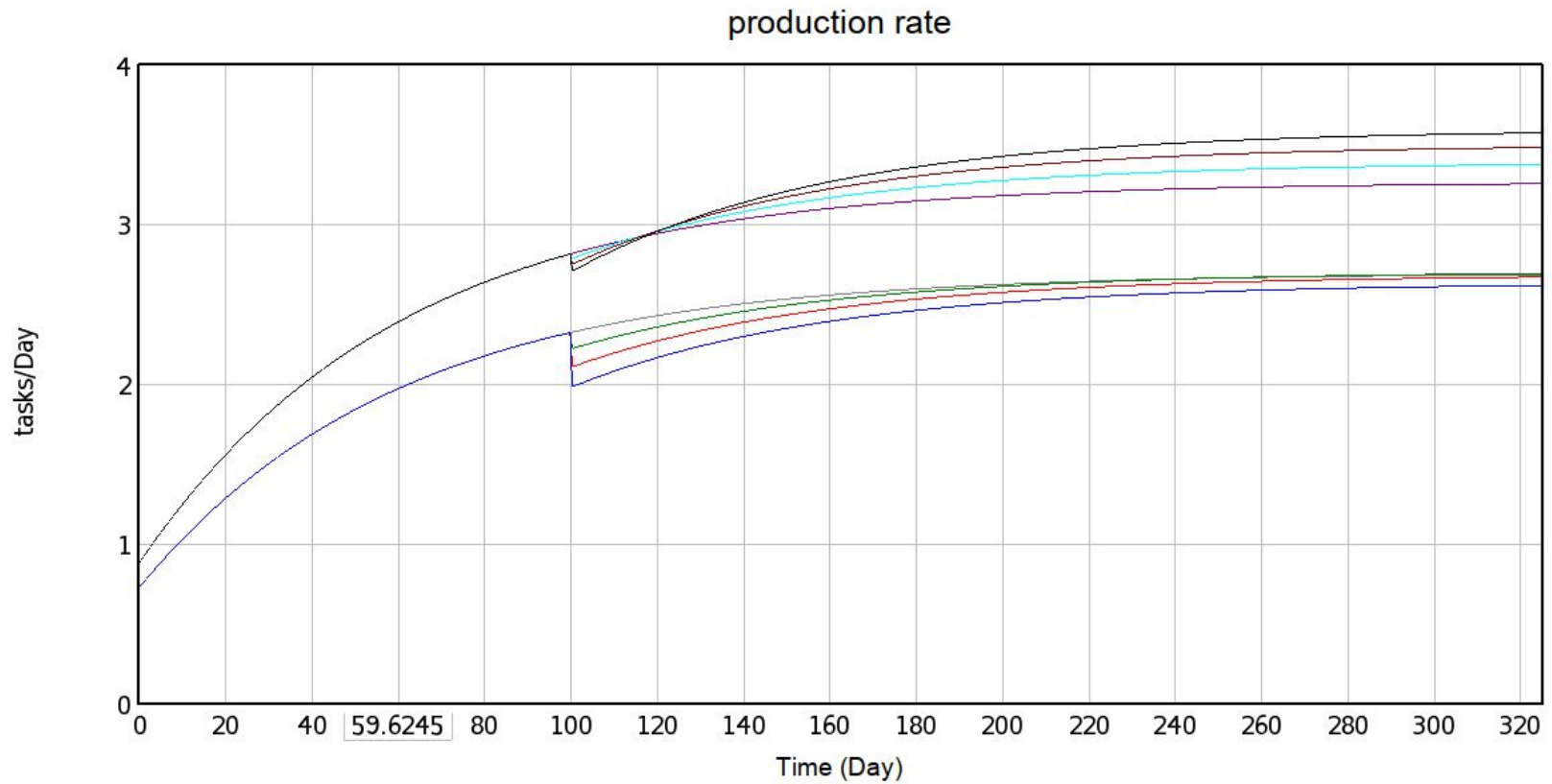
- ✓ Trial 8
- ✓ Trial 7
- ✓ Trial 6
- ✓ Trial 5
- ✓ Trial 4
- ✓ Trial 3
- ✓ Trial 2
- ✓ Trial 1

Legend for communication overhead graph:

- ✓ Trial 8
- ✓ Trial 7
- ✓ Trial 6
- ✓ Trial 5
- ✓ Trial 4
- ✓ Trial 3
- ✓ Trial 2
- ✓ Trial 1

# SBS Planning - Environment

## Output Analysis (SG25)



# Reporting Guidelines for SBS

Identification

Study Definition

**Context**

Problem

**Goals**

**Questions**

Hypotheses

**Justification for Simulation**

Background and Related Work

Simulation Model and its Validity

Participants

Experimental Design

Intermediate Runs

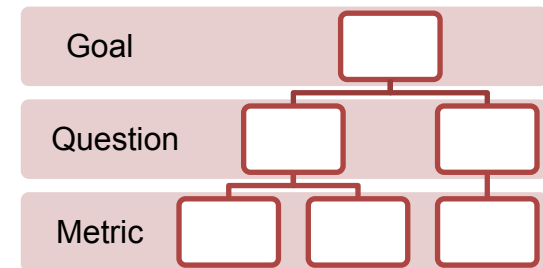
Supporting Data

Simulation Environment

Output Analysis

Threats to Validity

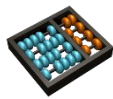
Conclusions and Future Work



**Extension from Balci (1999):**

*Cost, time and benefits*

*Observable phenomenon,  
high-order effects, risks, data  
availability.*



# Reporting Guidelines for SBS

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### Simulation Environment

### Output Analysis

### Threats to Validity

### Conclusions and Future Work

#### Procedure

Face Validity

Comparison to Reference Behaviors

Comparison to Other Models

Event Validity

Historical Data Validation

Rationalism

Predictive Validation

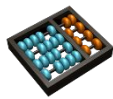
Internal Validity

Sensitivity Analysis

Testing model structure and behavior

Based on empirical evidence

Turing Tests



# Reporting Guidelines for SBS

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Supporting Data

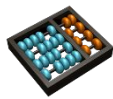
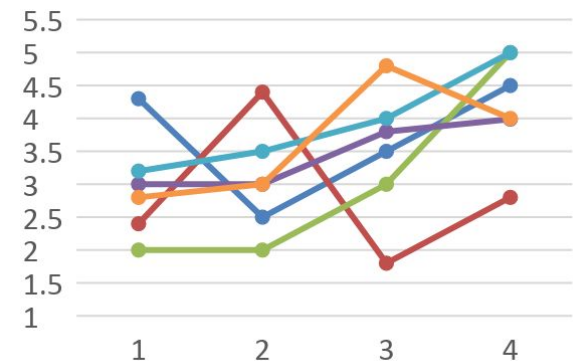
Simulation Environment

**Output Analysis**

**Threats to Validity**

Conclusions and Future Work

Scenario	Factor 1	Factor 2	...	Factor K
1	0	0	...	0
2	1	0	...	0
...	...	...	...	...
N	1	1	...	1





# Reporting Guidelines for SBS

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**Supporting Data**

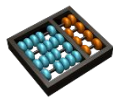
**Simulation Environment**

Output Analysis

Threats to Validity

Conclusions and Future Work

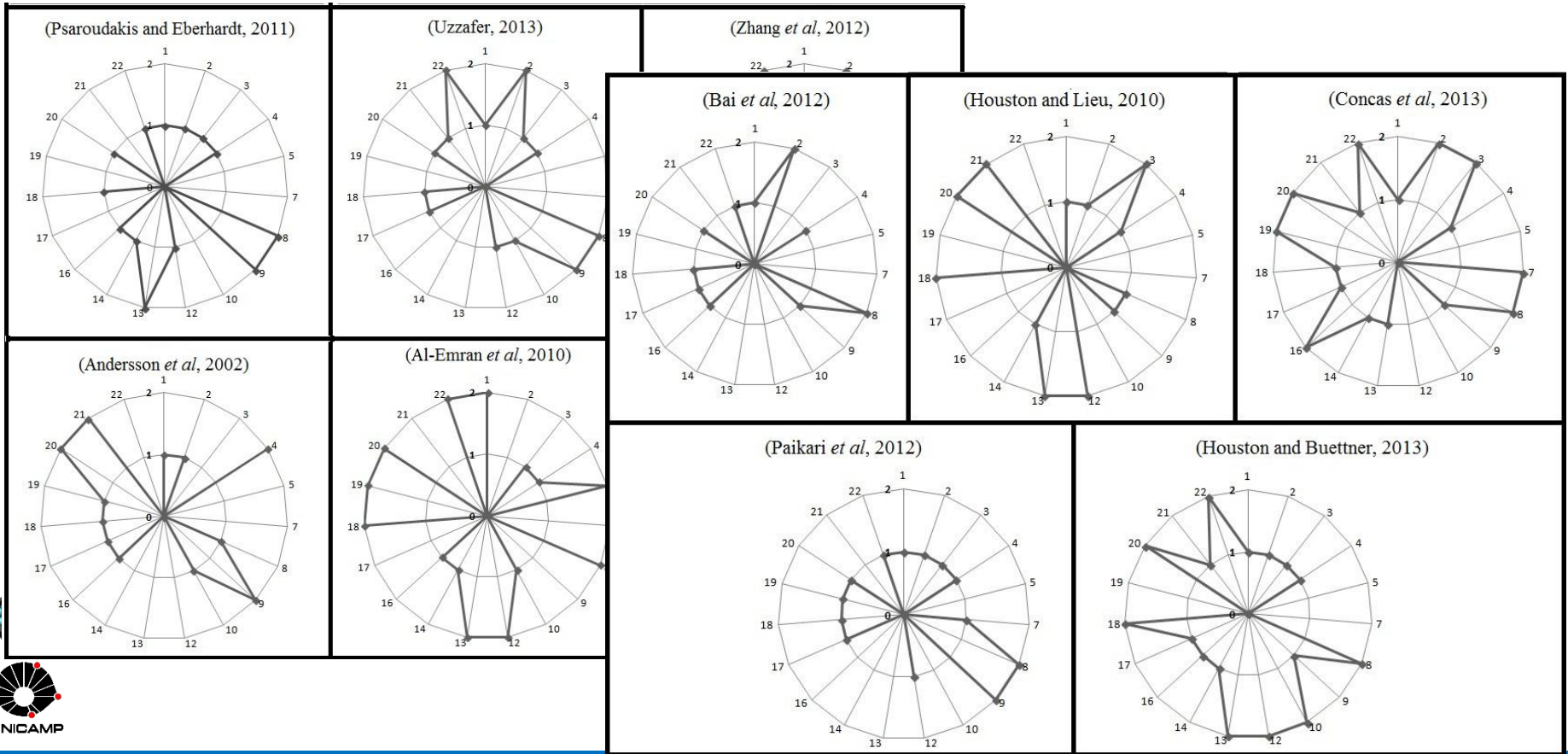
*Real or artificial?*



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# Reporting Guidelines for SBS

## Analysis against the literature



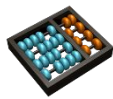
# *In Silico* Studies

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`breno@ic.unicamp.br`

# References

- Banks, J. Introduction to Simulation. In: Winter Simulation Conference (WSC'99). Phoenix, AZ, USA (1999)
- Alexopoulos, "Statistical analysis of simulation output: State of the art". Simulation Conference, 2007 Winter, 2007.
- Barros, M. O., Travassos, G. H. Contributions of In Virtuo and In Silico Experiments for the Future of Empirical Studies in Software Engineering. In: WSESE03. Fraunhofer IRB Verlag, Rome (2003)
- O. Balci, "Guidelines for successful simulation studies," Proc. Winter Simulation Conference, pp. 25-32, 1990.
- B. B. N. França, G. H. Travassos, "Are We Prepared for Simulation Based Studies in Software Engineering yet?," Proc. IX Experimental Software Engineering Latin American Workshop, Buenos Aires, Argentina, 2012.
- França, B.B.N.; Travassos, G.H. Reporting Guidelines for Simulation-Based Studies in Software Engineering. In: International Conference on Evaluation and Assessment in Software Engineering, EASE, Ciudad Real, Spain. 2012.
- Höst, M., Regnell, B., Tingström, C. A framework for simulation of requirements engineering processes EUROMICRO 2008 - Proceedings of the 34th EUROMICRO Conference on Software Engineering and Advanced Applications, SEAA 2008, 2008, 183-190
- Müller, M.; Pfahl, D. Simulation Methods. Guide to Advanced Empirical Software Engineering. 2008, Section I, 117-152, DOI: 10.1007/978-1-84800-044-5\_5



# References

- Ahmed, R.; Hall, T.; Wernick, P.; Robinson, S. & Shah, M. Software process simulation modelling: A survey of practice. Journal of Simulation, 2008, 2, 91 – 102.
- Zhang, H., Kitchenham, B., Pfahl, D.: Reflections on 10 years of software process simulation modeling: A systematic review. LNCS, vol. 5007, pp. 345-356 (2008)
- Birta, L.G.; Arbez, G. Modelling and Simulation: Exploring Dynamic System Behaviour. Springer. 2007.
- John A. Sokolowski; Catherine M. Banks. Principles of Modeling and Simulation: A Multidisciplinary Approach. John Wiley & Sons, Inc. 2009.
- Severance, F. L. System Modeling and Simulation: An Introduction. John Wiley & Sons, Inc. 2001.
- França, B.B.N.D. and Travassos, G.H., 2013. Are we prepared for simulation based studies in software engineering yet?. CLEI electronic journal, 16(1), pp.9-9.
- Ali, N.B., Petersen, K. and Wohlin, C., 2014. A systematic literature review on the industrial use of software process simulation. Journal of Systems and Software, 97, pp.65-85.

