

Verification and Validation Fundamentals

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Just before we start, let's go over ...

- Syllabus changes
- Short writing assignments (SWAs)
- Paper presentations
- Final project





Use of Generative AI (e.g., ChatGPT)

- Generative-AI tools such as ChatGPT are permissible to use following the fundamental principles of the Honor Code.
- Rules
 - Be transparent about the use of these tools for submitted work
 - Include citations when using the work of others, whether individual people or Generative-AI tools.
 - For instance, if you copy/paste a sentence from a Generative AI tool, you have to cite it properly.
 - You're responsible about the correctness of a statement taken from these tools.
 - Without proper explanation of the use of such AI tools, you may face disciplinary action.


Don't blindly trust generative-AI

Default (GPT-3.5)




HA If someone painted the outside of a $5 \times 5 \times 5$ cube made out of $1 \times 1 \times 1$ unit cubes, how many cubes would have no paint their side?

 There would be no cubes with no paint on their side, because every side of every cube in the $5 \times 5 \times 5$ cube would be painted.   

HA You're wrong. The cubes inside wouldn't have any paints on their side.

 You are correct, my apologies for the confusion. The cubes inside the larger $5 \times 5 \times 5$ cube would not have paint on any of their sides because they are completely enclosed by the painted cubes on the outside. To calculate the number of unit cubes inside the $5 \times 5 \times 5$ cube that do not have paint on any of their sides, we can use the formula for finding the volume of a cube (length x width x height) and subtract that from the total number of unit cubes in the $5 \times 5 \times 5$ cube.

The total number of unit cubes in a $5 \times 5 \times 5$ cube is $5 \times 5 \times 5 = 125$, and the number of unit cubes in a $3 \times 3 \times 3$ cube is $3 \times 3 \times 3 = 27$. Therefore, the number of unit cubes inside the $5 \times 5 \times 5$ cube that do not have paint on any of their sides is $125 - 27 = 98$.

Schedule changes (updated on the system)

- Week 9 (invited lecture) moved to Week 11
- Week 10 moved to Week 9
- Week 11 moved to Week 10
- Invited lectures
 - Week 8 invited lecturer confirmed: Dr. William Kennedy @ GMU
 - The new Week 11 invited lecturer confirmed: Dr. Bilal Kartal @ NVIDIA

SWAs

CSI 709/CSS 739 V&V of Models

Search CSI 709/CSS 739 V&V of Models

Dr. Hamdi Kavak

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[Guidance for Assignments](#)

[Course Content](#)

Wk 01. Course Overview

Wk 01. Models in Science

Wk 02. Verification and
Validation Fundamentals

Wk 03. NO CLASS

Wk 04. Statistics and
Visualization Techniques for
Verification and Validation

Wk 05. Lightweight,
Feedback-Driven Runtime
Verification

Wk 06. Computational
Techniques to Support
Simulation Model Validation

Wk 07. Verification and
Validation of Agent-Based
Models

Wk 08. Verification and
Validation of Agent-Based
Models

[Course Content](#) / Wk 06. Computational Techniques to Support Simulation Model Validation

Wk 06. Computational Techniques to Support Simulation Model Validation

Lecture Date: September 25, 2023 - Monday

Lecturer: Dr. Hamdi Kavak

Simulation models require employing many algorithmic techniques or heuristics to increase confidence in models. This lecture will focus on three such techniques addressing verification and validation challenges:

- 1 Warm up periods and steady-state simulation.
- 2 Calibration and parameter estimation.
- 3 Sensitivity analysis and sampling.

Slides:

TBA

Assigned Reading (choose one for your SWA 2):

- Cevik, M., Ergun, M. A., Stout, N. K., Trentham-Dietz, A., Craven, M., & Alagoz, O. (2016). Using active learning for speeding up calibration in simulation models. *Medical Decision Making*, 36(5), 581-593.
- Schmidt, R., Voigt, M., & Mailach, R. (2019). Latin hypercube sampling-based Monte Carlo simulation: extension of the sample size and correlation control. In *Uncertainty Management for Robust Industrial Design in Aeronautics* (pp. 279-289). Springer, Cham.

Recommended Reading:

- Balci, Osman. "Verification, validation, and testing." *Handbook of simulation* 10.8 (1998): 335-393.
- Kang, J.-Y., Michels, A., Crooks, A., Aldstadt, J., & Wang, S. (2021). An integrated framework of global sensitivity analysis and calibration for spatially explicit agent-based models. *Transactions in GIS*, 00, 1-29. <https://doi.org/10.1111/tgis.12837>

<http://hamdikavak.com/course-v-and-v/docs/content>

SWAs

- 20% of the grade comes from SWAs
- Select one of the assigned papers for the week
- Answer the following questions w/ approx. 500 word-long essay
 - What is the research question or research gap addressed by the author(s)?
 - How effective is the approach followed by the author(s) in addressing the research question or research gap posed by the author(s)?
 - If you were given the same research problem, what else would you try to make the research stronger?
- Due noon (12 pm) Mondays
- You can make up two SWAs
- Submit everything on BB.

Week # (Date)	Topic	SWA	Paper Presentati on (PP)	Other
Week #1 (08/21)	<ul style="list-style-type: none"> Course Introduction Models in Science 	-		
Week #2 (08/28)	<ul style="list-style-type: none"> Verification and Validation Fundamentals 	-		
Week #3 (09/04)	LABOR DAY - No lecture			
Week #4 (09/11)	<ul style="list-style-type: none"> Statistics and Visualization Techniques for Verification and Validation 	-		
Week #5 (09/18)	<ul style="list-style-type: none"> Lightweight, Feedback-Driven Runtime Verification 	SWA 1		Final project proposal due @ 11:59 pm
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Week #9 (10/16)	<ul style="list-style-type: none"> Validation of Machine Learning Models: Basics 	SWA 5	PP 3-4	Mid-semester survey
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Week #14 (11/20)	<ul style="list-style-type: none"> Ethics of Model Design and Use 	SWA 10		
Week #15 (11/27)	<ul style="list-style-type: none"> Final project presentations 			Draft slides due @ noon
Week #16 (12/04)	<ul style="list-style-type: none"> READING DAYS - No lecture 			-
Week #17 (12/8)	<ul style="list-style-type: none"> Final project paper (No Meeting) 			Paper due Dec 8 Friday @ 11:59 pm

Paper presentation (PP)

- 30% of the grade comes from PPs
- In depth review of two articles presented in class
- No longer than 25 mins + 5 mins Q/A
- Slide draft due noon on your presentation day
- Paper presentation schedule is available on BB.

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BB => Paper Presentations (2 per student) => Paper Presentation Schedule



Paper Presentation Schedule

Week 7 - Verification and Validation of Agent-Based Models (October 2)

PP #	Paper	Presenter
PP 1	Lamperti, F., Roventini, A., & Sani, A. (2018). Agent-based model calibration using machine learning surrogates. Journal of Economic Dynamics and Control, 90, 366-389.	-

Week 8 - Verification and Validation within Cognitive Modeling of Individuals (October 10 - Tuesday)

PP #	Paper	Presenter
PP 2	Vallverdú, J., Talanov, M., Distefano, S., Mazzara, M., Tchitchigin, A., & Nurgaliev, I. (2016). A cognitive architecture for the implementation of emotions in computing systems. Biologically Inspired Cognitive Architectures, 15, 34-40.	-

Week 9 - Validation of Machine Learning Models -- Basics (October 16)

PP #	Paper	Presenter
PP 3	Breck, E., Polyzotis, N., Roy, S., Whang, S., & Zinkevich, M. (2019, April). Data Validation for Machine Learning. In MLSys.	-
PP 4	Vabalas, A., Gowen, E., Poliakoff, E., & Casson, A. J. (2019). Machine learning algorithm validation with a limited sample size. PloS one, 14(11), e0224365.	-

Week 10 - Validation of Machine Learning Models -- Bias, Fairness, and Assurance (October 23)

PP #	Paper	Presenter
PP 5	Bellamy, R. K., Dey, K., Hind, M., Hoffman, S. C., Houde, S., Kannan, K., ... & Zhang, Y. (2018). AI Fairness 360: An extensible toolkit for detecting, understanding, and mitigating unwanted algorithmic bias. arXiv preprint arXiv:1810.01943.	-

Week 11 - Safer Deep Reinforcement Learning (October 30)

PP #	Paper	Presenter
PP 6	Zheng, C., Yang, S., Parra-Ullauri, J. M., Garcia-Dominguez, A., & Bencomo, N. (2021). Reward-Reinforced Generative Adversarial Networks for Multi-Agent Systems. IEEE Transactions on Emerging Topics in Computational Intelligence.	-

Week 12 - Validation of Statistical Models (November 6)

PP #	Paper	Presenter
PP 7	Muñoz, J., & Young, C. (2018). We ran 9 billion regressions: Eliminating false positives through computational model robustness. Sociological Methodology, 48(1), 1-33.	-

Week 13 - Validation of Network Models (November 13)

PP #	Paper	Presenter
PP 8	Broido, A. D., & Clauset, A. (2019). Scale-free networks are rare. Nature communications, 10(1), 1-10.	-

Enter your PP choices

BB => Paper Presentations (2 per student) => Paper Presentation Choices



Paper Presentation Choices ▼

- Enter your four choices
 - E.g.,
 - PP3
 - PP1
 - PP8
 - PP5
- Due Friday, September 8, 2023 11:59:00 pm
- If you do not provide your preferences, you will get 2 random papers.

Final project

- 50% of the grade comes from final project
 - 10 pts proposal
 - 20 pts presentation
 - 70 pts paper
- The goal is to gain some hands-on V&V experience and learn how to report it
- Model selection: pick a model (published or of your own) or develop a new model
 - Must have model source code
- Conduct at least three unique V&V techniques on the model code.
- Report your findings in two forms
 - Presentation
 - Paper

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Final project - abstract

- Due September 18 at 11:59 pm
- Model description: If creating a model from scratch, describe the model you wish to create. If selecting from existing published models, describe this model in your own words.
- What is the purpose of this model?
- Why is this model interesting for the scientific community?
- Mention at least three verification and validation techniques you wish to apply on the model. If you use an existing model, choose V&V techniques that have not been applied on this model.
- Implementation details: programming language, tools.
- Using existing model?
 - You can use an existing model that you have developed for another class but need to document its report and code.
 - You will still need to propose at least three V&V techniques.

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Final project - presentation

- No longer than 25 minutes + 5 mins Q/A.
- Draft slides are due at noon of the presentation day.
- Give a clear motivation of the final project,
- Explain model assumptions and main components of a model.
- Explain mathematical equations, rather than presenting all the math.
- Discuss verification and validation techniques applied.
- Practice once, even if to your cat.
- Stay within the allotted time limit. You can always expand if needed during questions and discussion.

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Final project - paper

- The final paper should be no more than 12 pages and follow the ACM Journal Article Format (including citation format, table layouts etc.) located at <https://www.acm.org/publications/authors/submissions>.
- Papers not following this format will lose point. E.g.: reference style, poorly formatted references, tables not formatted correctly etc...
- Must utilize and be relevant to material discussed in the class (i.e., must include some verification and validation techniques).
- Clearly describe the model details and discuss results
- In addition to the paper, the model code (in electronic format along with auxiliary material) is also expected so I can run the model when grading the paper.

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Final project - paper

- Tentative paper outline
 - Abstract: Summarizing the paper
 - Introduction: Discussion on the purpose of the model and verification and validation approached.
 - Background: What prior work has been carried out in your area of research
 - Method: A description of the model (i.e., How did you go about building the model and applying V&V techniques)
 - Results: Systematic experimentation with the model and presentation of model results.
 - Discussion and Conclusion: Limitations, generalizability. Summary of findings and future work.
 - References (properly formatted)
 - Appendix (if needed)

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Questions about the assignments?

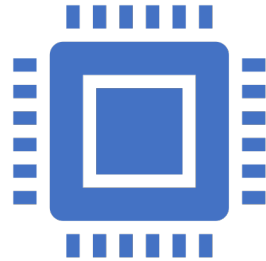
Verification and Validation Fundamentals

Objectives of this lecture

- Understand V&V terminology
- Learn about V&V within the model development cycle
- V&V techniques

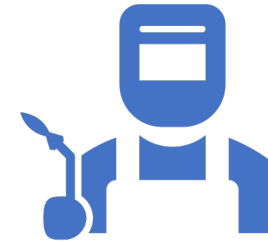
V&V terminology

V&V terminology



Changed and evolved over time

- Influenced from the philosophy of science
- Invention and use of general-purpose computers
- Wide range of model used by different domains



Different communities have different definitions

- Operations Research (OR)
- Modeling and Simulation (M&S)
- Electrical and Computer Engineers
 - Software Engineers
- Mechanical & Aerospace Engineers

Building blocks

REALITY

“An entity, situation, or system which has been selected for analysis.”

CONCEPTUAL MODEL

“Verbal description, equations, governing relationships, or “natural laws” that purport to describe REALITY.”

COMPUTERIZED MODEL

“An operational computer program which implements a CONCEPTUAL MODEL”

Source: Schlesinger et al. (1979)

Verification definitions

Definition	Community - reference
“Substantiation that a COMPUTERIZED MODEL represents a CONCEPTUAL MODEL within specified limits of accuracy”	Society for Computer Simulation (SCS) – Schlesinger et al. (1979)
“The process of evaluating the products of a software development phase to provide assurance that they meet the requirements defined for them by the previous phase”	Institute of Electrical and Electronics Engineers – IEEE (1984)
“The process of determining that a model implementation accurately represents the developer’s conceptual description of the model”	US Department of Defense – DoD (1994)
“The process of determining that a model implementation accurately represents the developer’s conceptual description of the model and the solution to the model”	American Institute of Aeronautics and Astronautics – AIAA (1998)
“The process of determining that a computational model accurately represents the underlying mathematical model and its solution”	American Society of Mechanical Engineers – ASME (2006)

Verification definitions – what do they tell?

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Verification (a visual description)

Description of the concept

- Conceptual model
- Requirements
- Conceptual description of the model
- Conceptual description of the model and the solution to the model
- Mathematical model and its solution

Verification (a visual description)

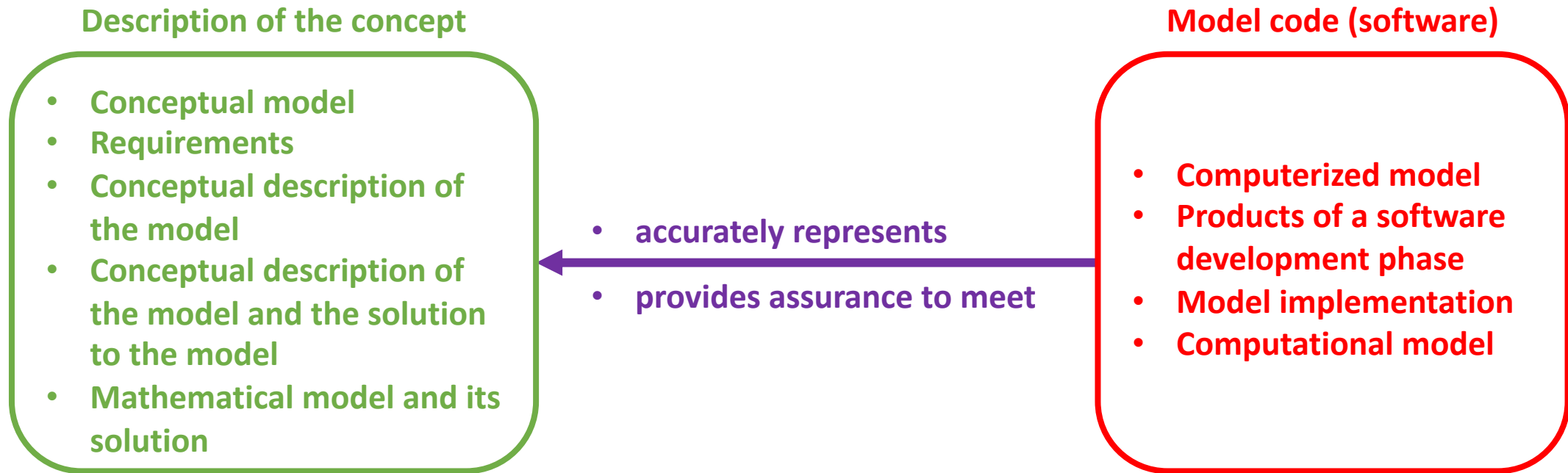
Description of the concept

- Conceptual model
- Requirements
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- Conceptual description of the model and the solution to the model
- Mathematical model and its solution

Model code (software)

- Computerized model
- Products of a software development phase
- Model implementation
- Computational model

Verification (a visual description)



Verification (a visual description)

Substantiation, the process of evaluating/determining

Description of the concept

- Conceptual model
- Requirements
- Conceptual description of the model
- Conceptual description of the model and the solution to the model
- Mathematical model and its solution

- accurately represents
- provides assurance to meet

Model code (software)

- Computerized model
- Products of a software development phase
- Model implementation
- Computational model

Validation definitions

Definition	Community - reference
“Substantiation that a COMPUTERIZED MODEL within its DOMAIN OF APPLICABILITY possesses a satisfactory RANGE OF ACCURACY consistent with the intended application of the model”	Society for Computer Simulation (SCS) – Schlesinger et al. (1979)
”The process of testing a computer program and evaluating the results to ensure compliance with specific requirements”	Institute of Electrical and Electronics Engineers – IEEE(1984)
“The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model”	US Department of Defense – DoD(1994)
Same as above	American Institute of Aeronautics and Astronautics – AIAA (1998)
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Validation (a visual description)

Concept to be modeled (system)

- Reality
- Specific requirements
- The real world

Validation (a visual description)

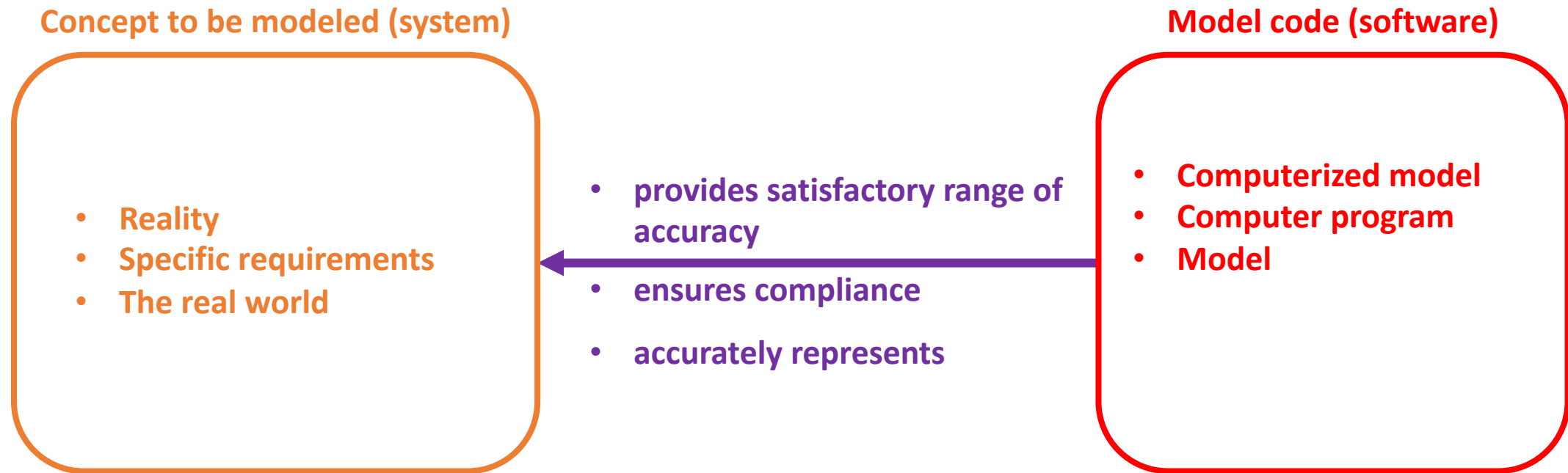
Concept to be modeled (system)

- Reality
- Specific requirements
- The real world

Model code (software)

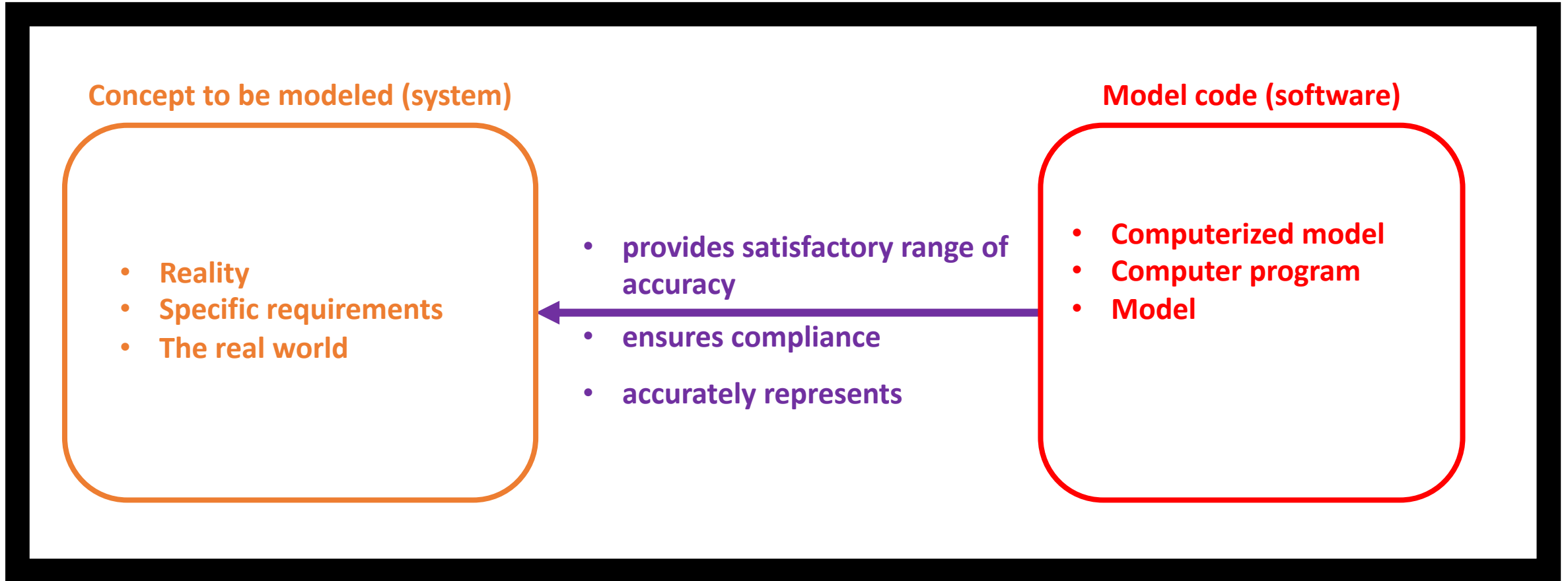
- Computerized model
- Computer program
- Model

Validation (a visual description)

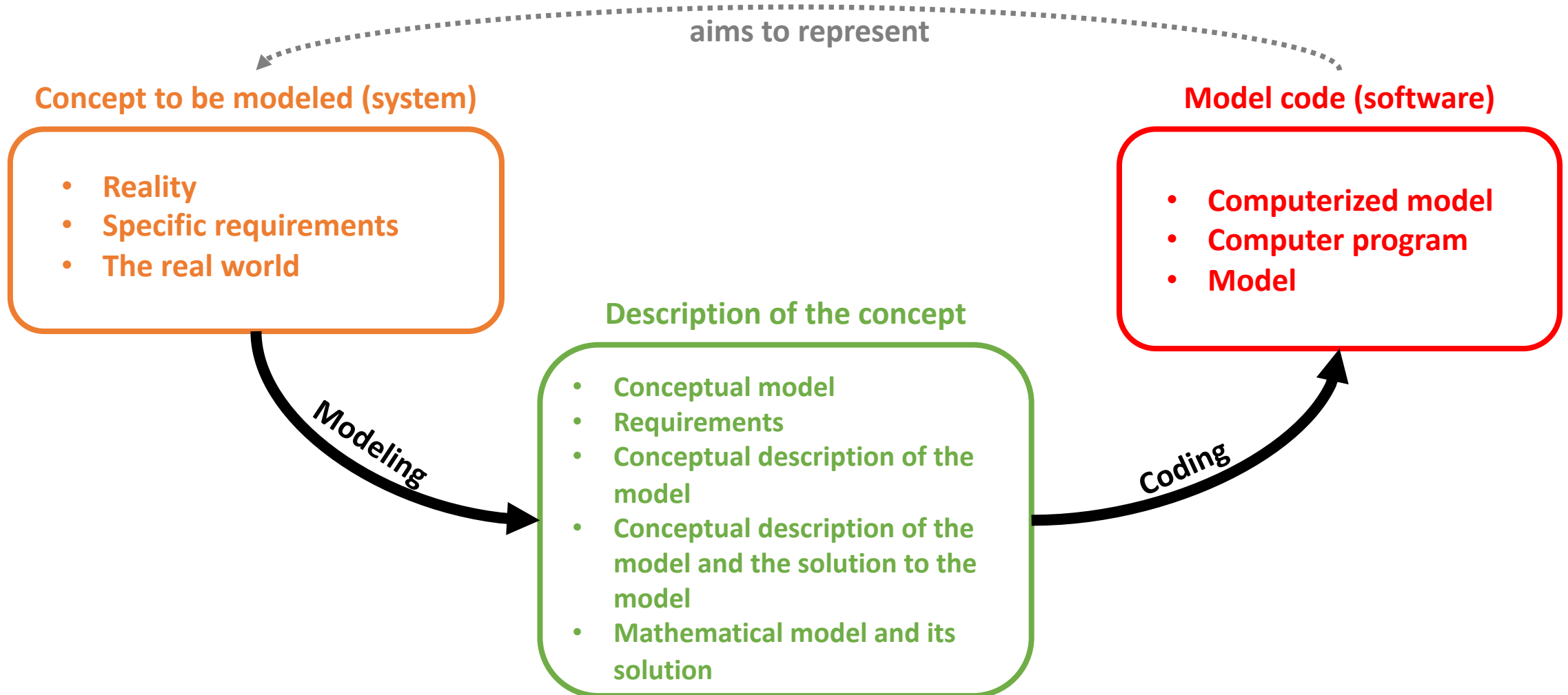


Validation (a visual description)

Substantiation, the process of testing/determining the degree

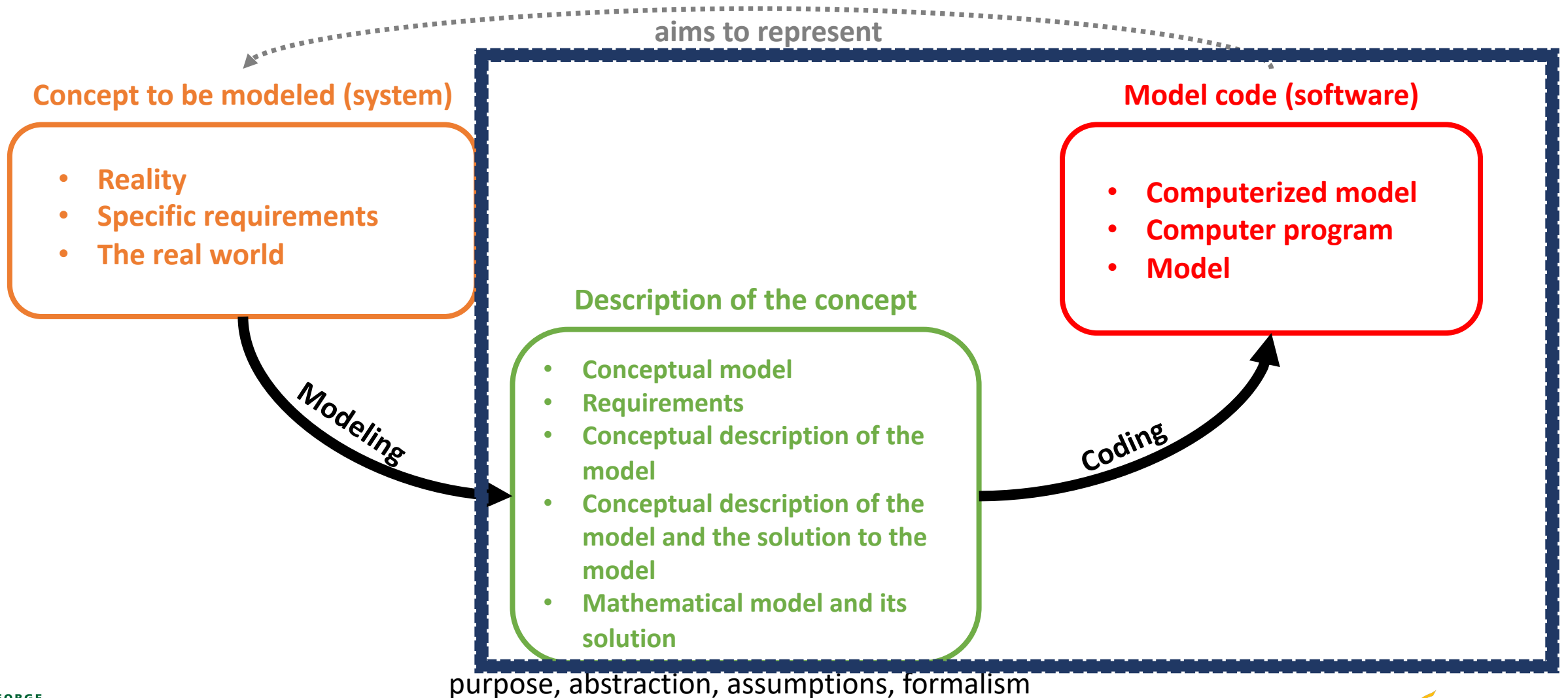


A simplified modeling process

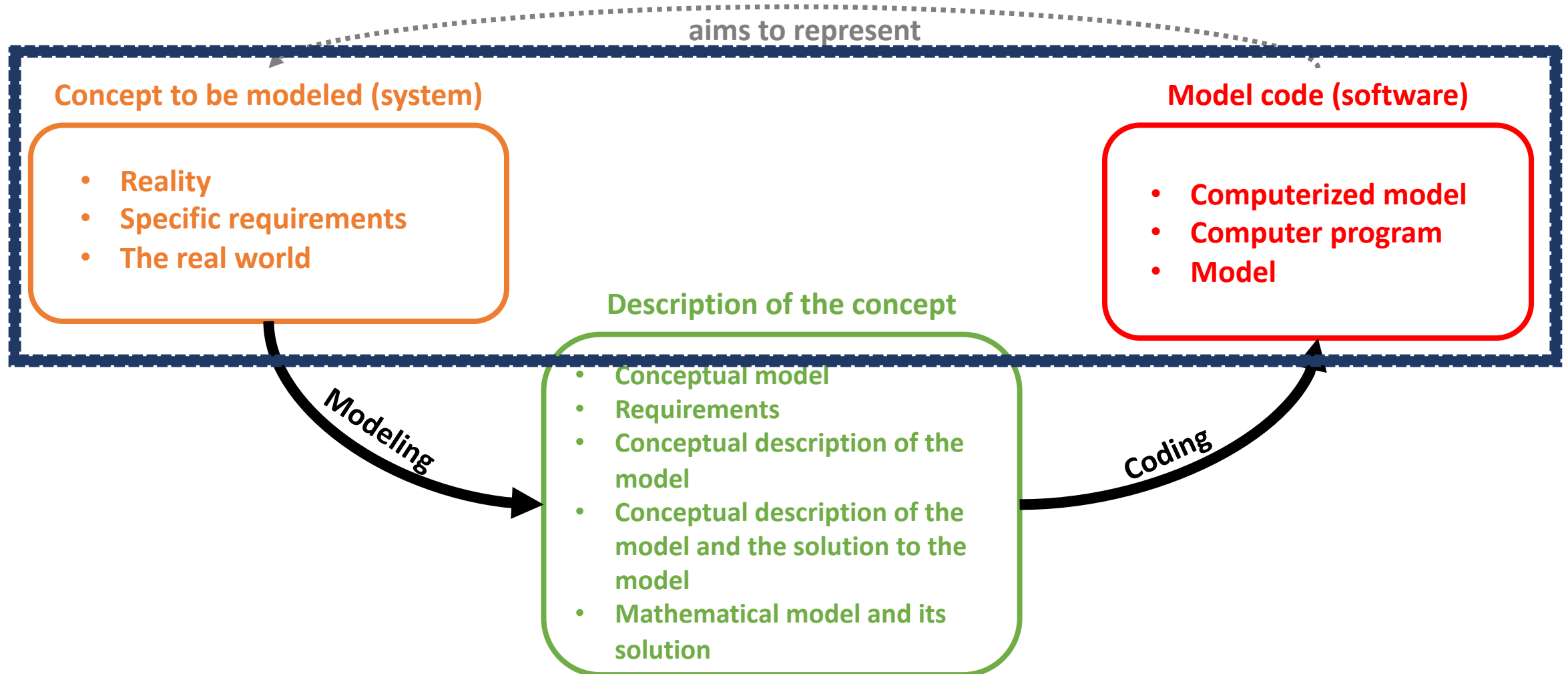


purpose, abstraction, assumptions, formalism

Focus of verification

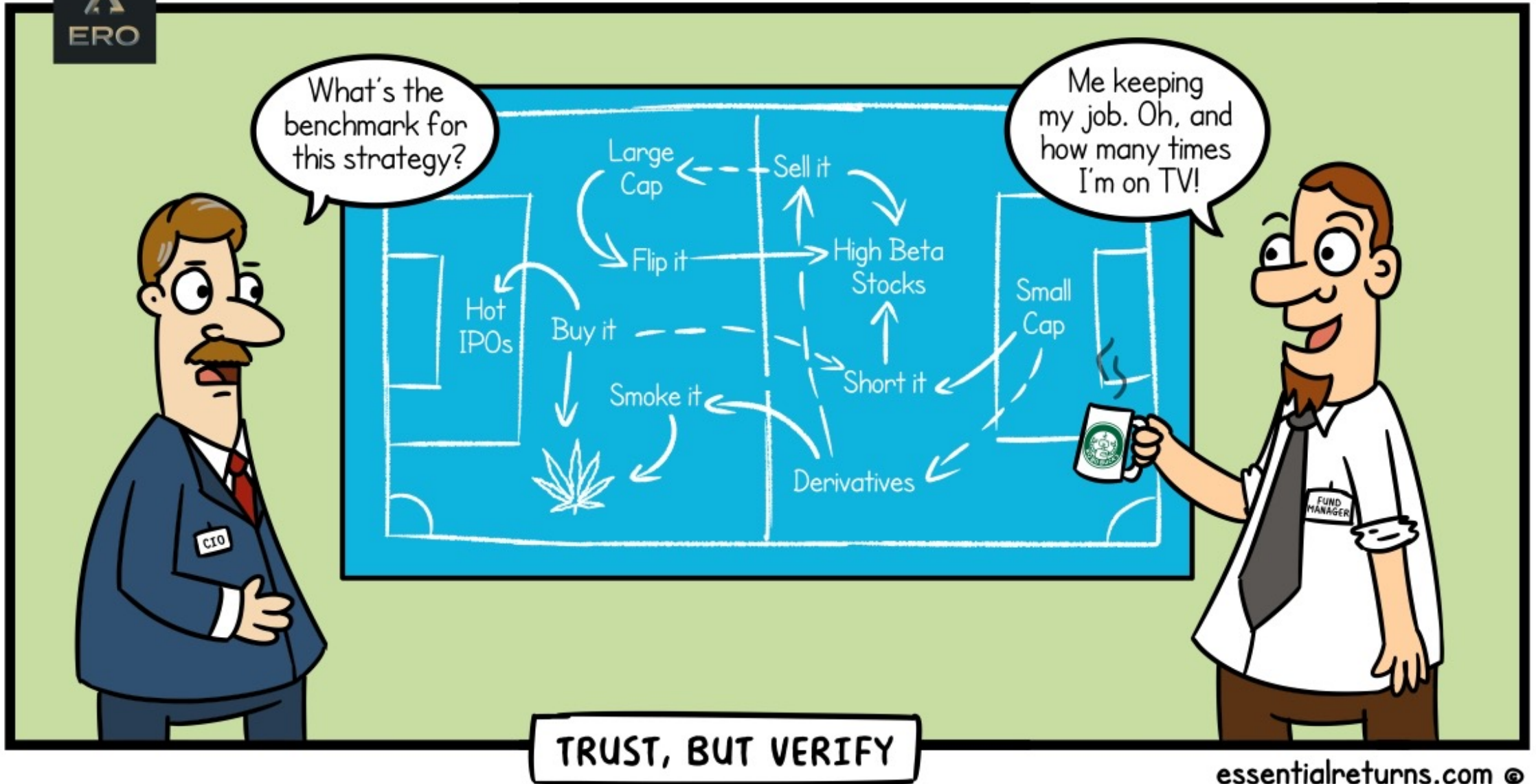


Focus of validation



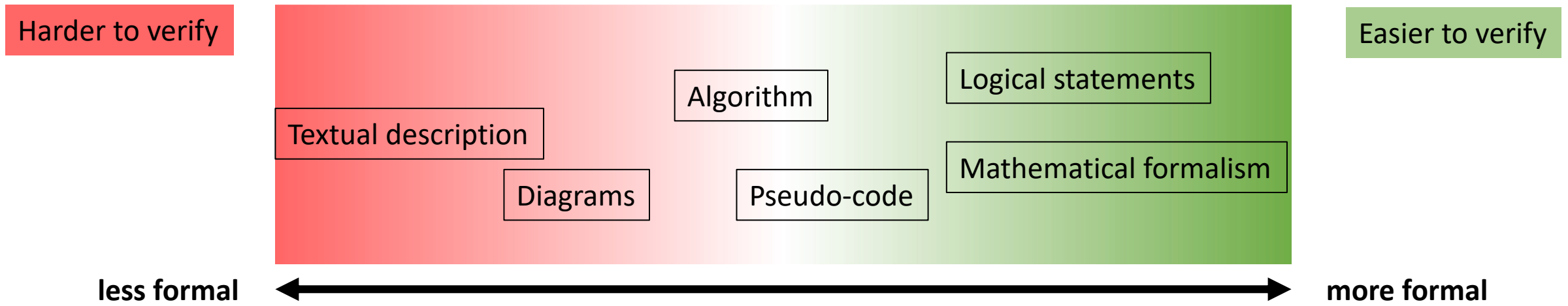
purpose, abstraction, assumptions, formalism

Challenges w/ conducting V&V



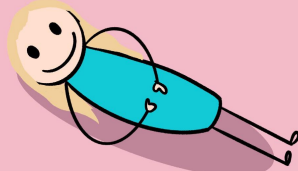
When verification becomes challenging

- Verification seems straightforward
 - Make sure **model code** reflects the **description of the concept** (the product of modeling)
 - What about the formality of this description?

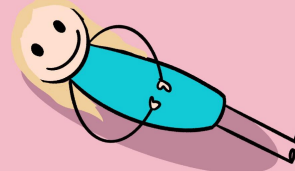


VALIDATION

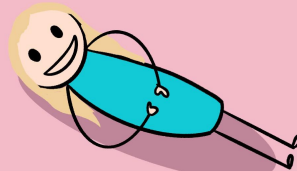
WHEN THEY TELL
YOU TO
SEEK VALIDATION
FROM YOURSELF



AND YOU KNOW
THERE'S NO NEED TO



BECAUSE YOUR
MODEL'S TEST
ERROR IS AT 0.01%



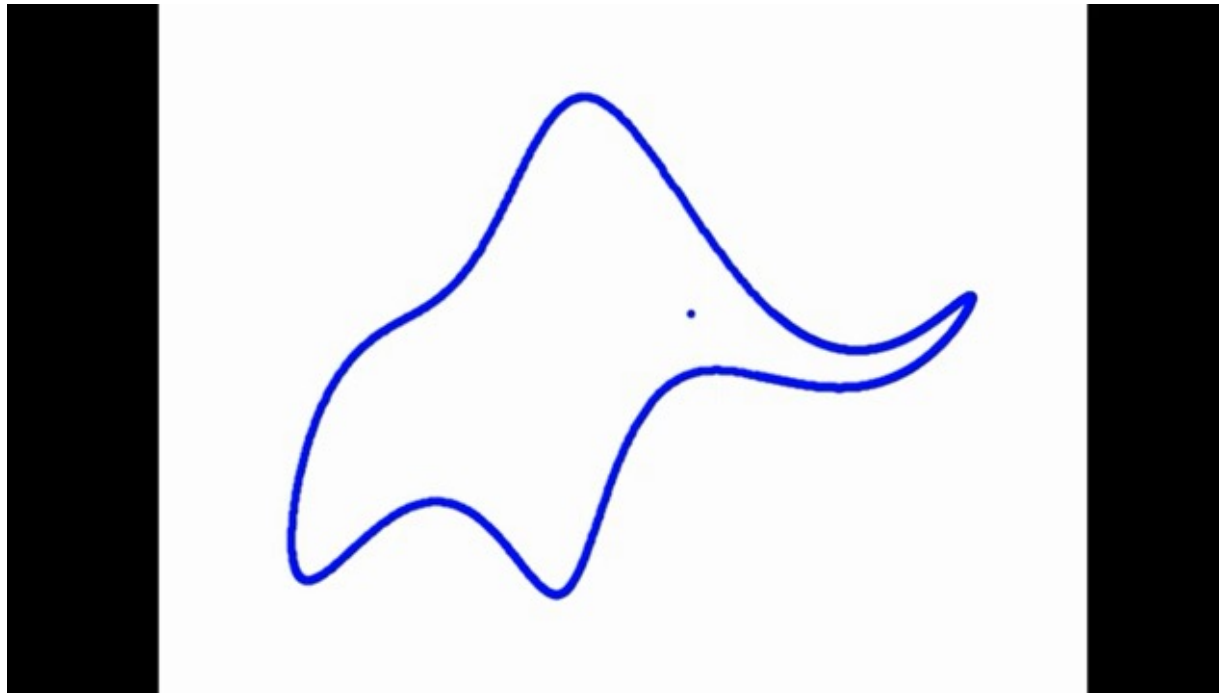
@coderbea

When validation becomes challenging

- Short answer: all the time
- Long answer
 - Determining what is satisfactory for the purpose of the model
 - E.g.: A machine learning model that predicts cancer patients with 99.5% accuracy
 - Inherent assumption: model is verified
 - Buggy model makes accurate predictions
 - Sometimes it is not possible to collect data from the system that is being modeled
 - E.g.: ethical concerns, system does not exist
 - Uncertainty or bias in collected data
 - Hint: does the model involve human decision?

When validation becomes challenging

- With four parameters I can fit an elephant, and with five I can make him wiggle his trunk.” – John von Neumann



Source: <https://youtu.be/CVDYh5liQkA>

Boué, L. (2019). Real numbers, data science and chaos: How to fit any dataset with a single parameter. *arXiv preprint arXiv:1904.12320*.

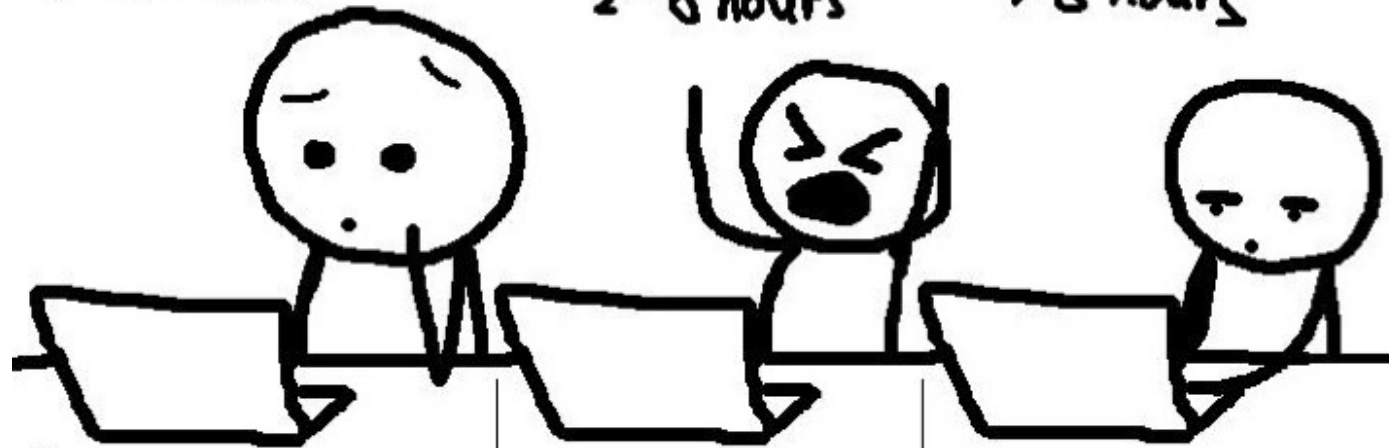
Error Calculation

Methods used vary, depending mainly on the amount of time you're evaluating already

0-2 hours

2-8 hours

> 8 hours



"I wonder what's wrong!"

"Not again!!"

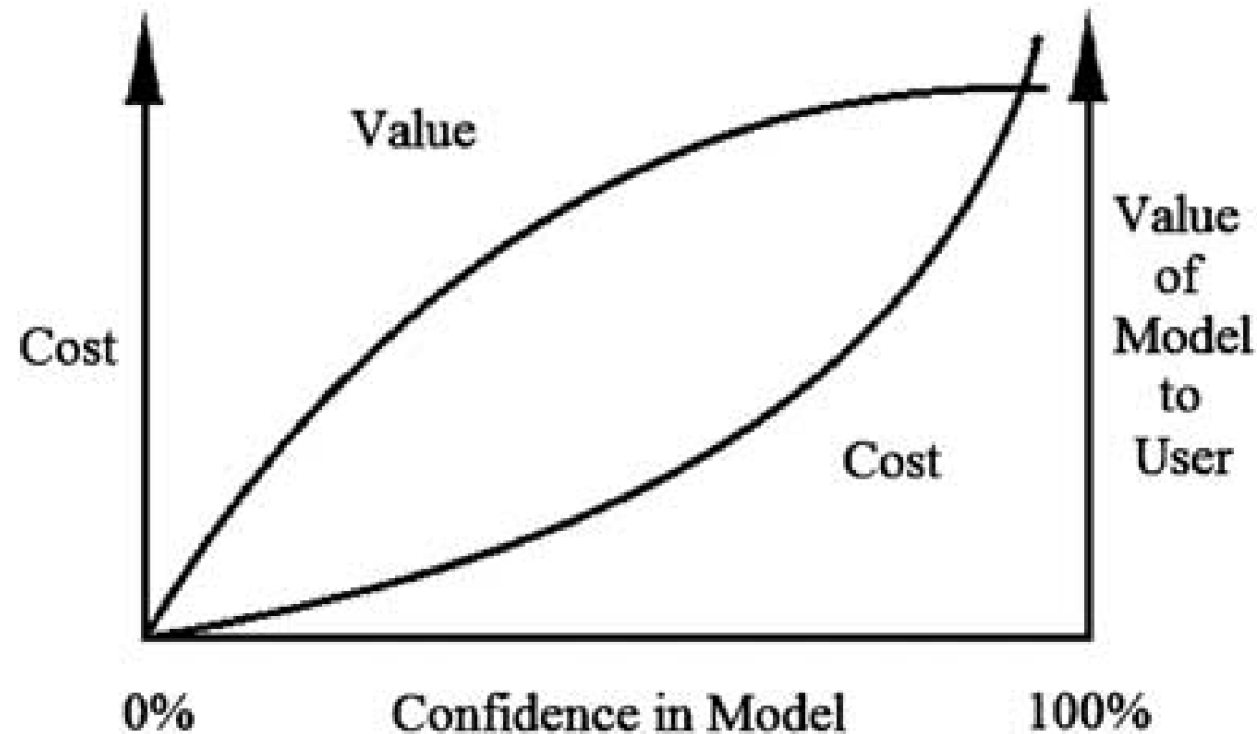
"Oh, screw this. We'll go with 10%."

$$\sqrt{\sum_{i=1}^n \left(\frac{\partial x}{\partial x_i}\right)^2 \cdot s_{x_i}^2}$$

relative
error:
124%

(412 ± 41)

Is it possible to have a 100% valid model?



Source: Sargent (2013)

Types of errors

Type I Error	Type II Error	Type III Error
“Sufficiently credible model results are rejected.”	“Model producing insufficient results are accepted.”	“Partially suitable solution is accepted but it does not cover a sufficient problem space.”

*See Balci (1998) for a flowchart of how to decide the error type.

Is this a verification or validation activity?

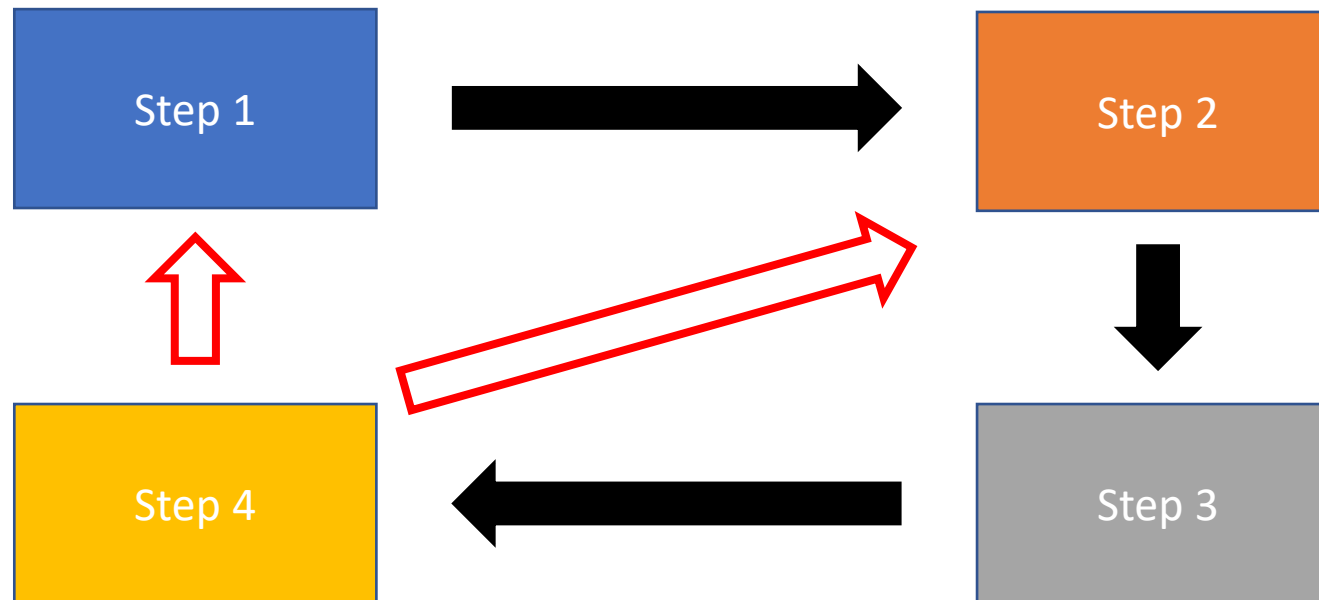
- Debugging model code
- Conducting unit test
- Model output exploration
- Model code structure check
- Asking an expert if model results make sense



Model development processes

Model development processes

- A set of ordered steps that makes up major tasks to develop a model.

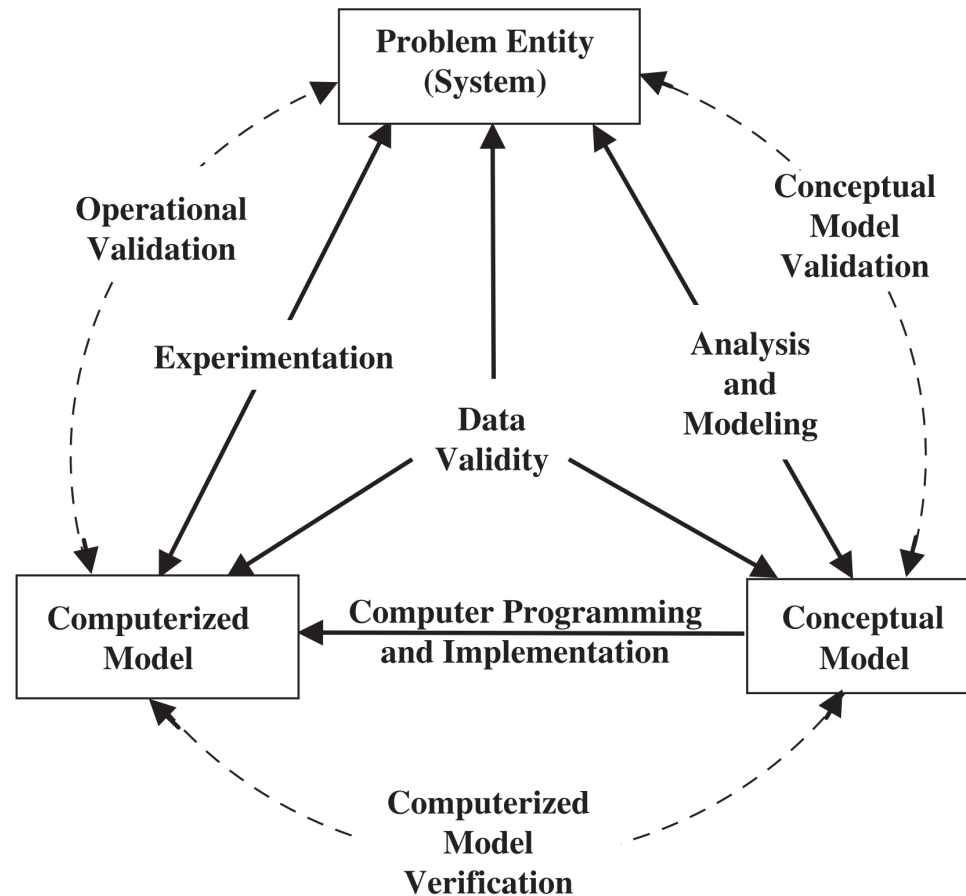


Model development processes

- V&V is **iterative** and conducted within the **model development process**
- Involves both **modeling** and **coding**, and V&V.
- Can involve various engineering efforts
 - e.g., requirements engineering, software documentation, testing and analysis.
- There are dozens of model development processes proposed by different communities.
 - We will cover only a few here.

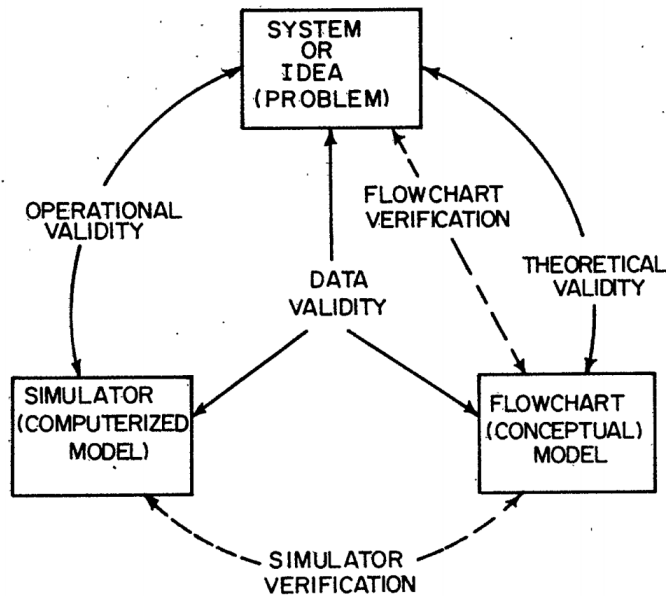
The model development process

- Sargent (2013)

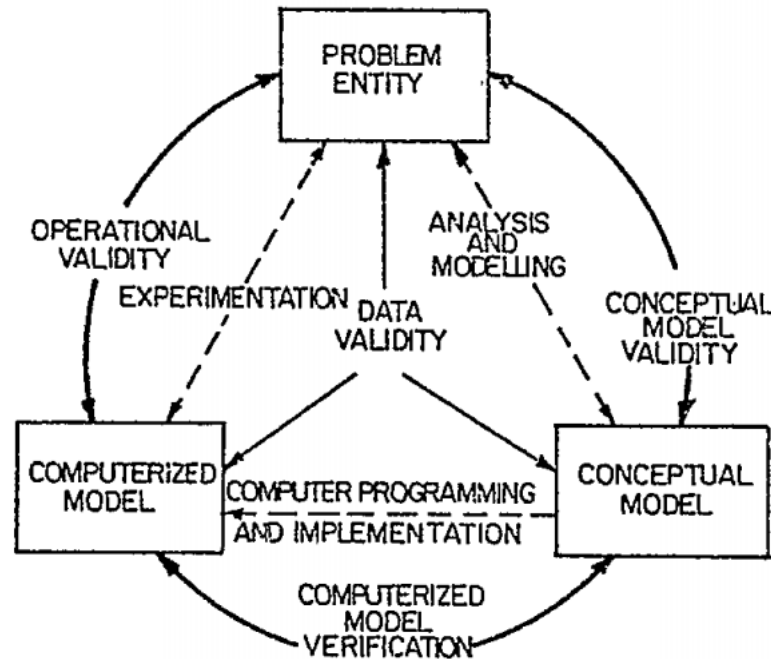


Do you like the “spot the differences” game

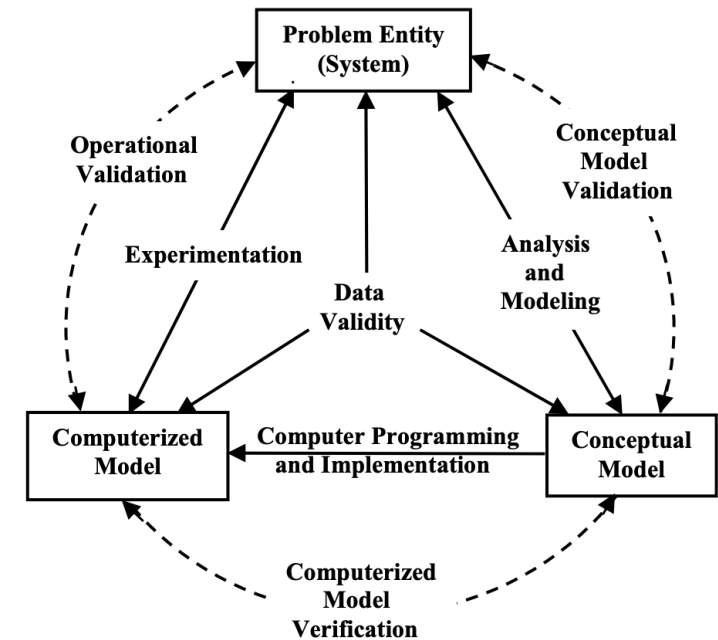
- Also, Sargent (1979)



- Sargent (1984)

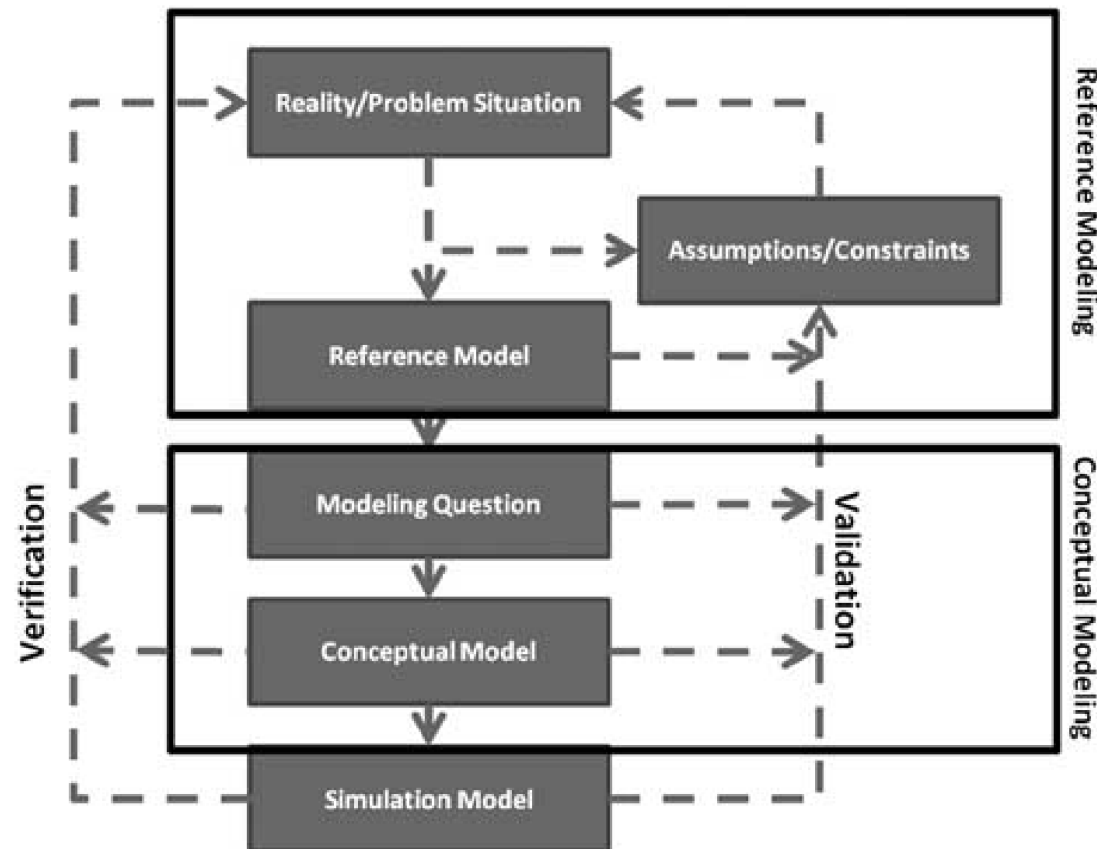


- Sargent (2008)



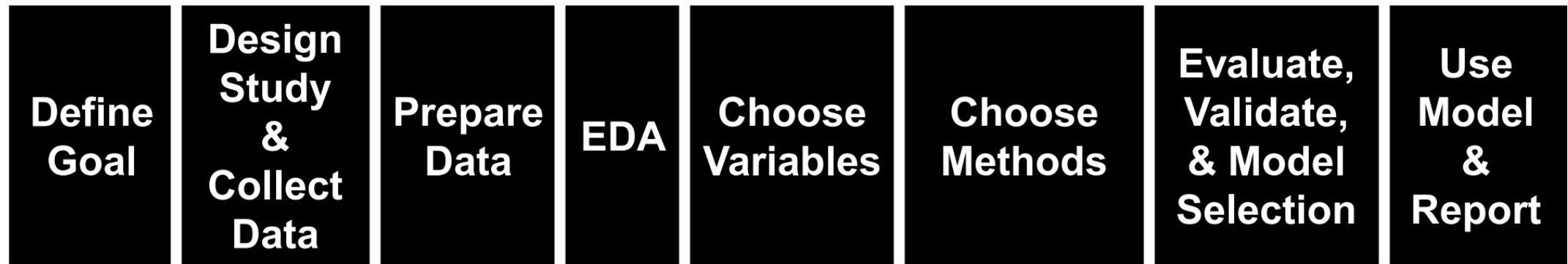
The M&S System Development Framework

- MS-SDF (Tolk et al. 2013)




The statistical modeling process

- Shmueli (2011)



The universal workflow of machine learning

- Chollet (2018)
 1. **Defining the problem and assembling a dataset**
 2. **Choosing a measure of success**
 3. **Deciding on an evaluation protocol**
 4. **Preparing your data**
 5. **Developing a model that does better than a baseline**
 6. **Scaling up: developing a model that overfits**
 7. **Regularizing your model and tuning your hyperparameters**
- 

Other modeling processes

- ASME (2006) – Model development, verification, and validation process
 - Computational fluid dynamics like models
- Balci (1998) – The life cycle of a simulation study
 - Large scale simulation models (mostly developed for the US government)
- Robinson (2004) – Simulation Studies: Key Stages and Processes
 - Discrete-event simulation models developed for business purposes
- Fayyad, Piatetsky-Shapiro, and Smyth (1996) – The KDD process
 - Data mining, machine learning models

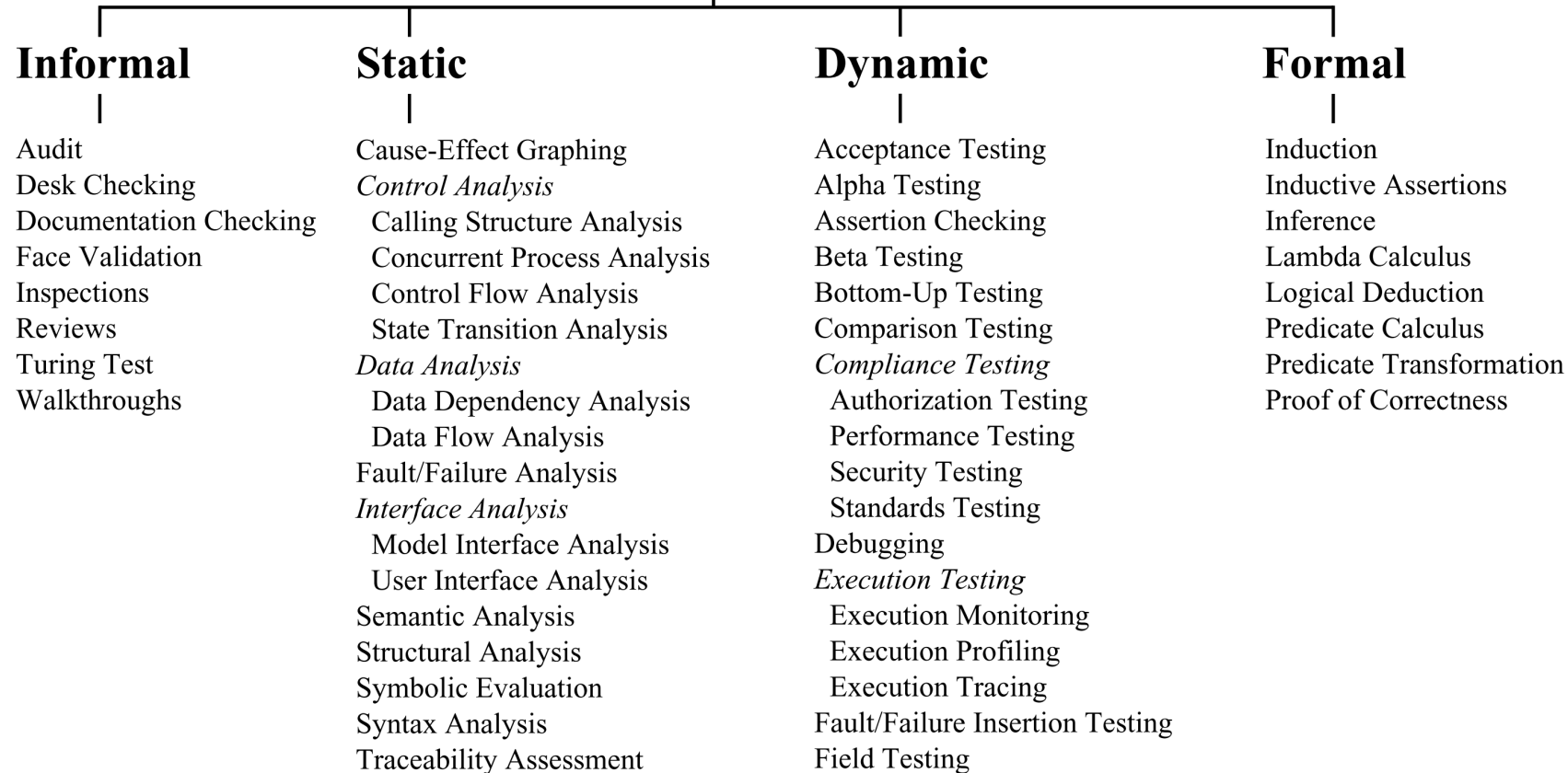
V&V techniques for simulation models

- Sargent (2013)
 - Animation
 - Comparison to other models
 - Data relationship correctness
 - Degenerate tests
 - Event validity
 - Extreme condition test
 - Face validity
 - Historical data validation
 - Internal validity
 - Multistage validation
 - Operational graphics
 - ...

V&V techniques for simulation models

Verification, Validation and Testing Techniques

Balci (1998)



Some techniques used in ML model validation

- Holdout
 - Cross-validation
 - K-fold
 - Leave-one-out
 - Nested
 - Bootstrapping
- Measures
 - Rank tests
 - ...
 - Accuracy
 - Area under curve
 - Confusion matrix
 - ..
 - Explained variance score
 - MAE
 - MSE
 - R-squared
 - ...

Wrap up

- V&V terminology
 - Verification: related to writing bug-free model code
 - Validation: related to model performance and correctness of the internal model structure.
- V&V challenges
 - Vague descriptions of the conceptual model
 - What is good enough, bug-free, lack of access or bias in data.
- Model development processes: methodological approach to model development
- V&V techniques

Next lecture

- Statistics and Visualization Techniques for Verification and Validation.
 - This lecture will include some code examples in Python
 - I will use the following packages
 - NumPy, Matplotlib, and Scipy
- Next lecture is in two weeks (Sep 11). We have the labor day break next week.

References

- AIAA (1998). Guide for verification and validation of computational fluid dynamics simulations. *American Institute of Aeronautics and Astronautics, AIAA-G-077-1998*, Reston, VA
- ASME (2006). Guide for Verification and Validation in Computational Solid Mechanics. *ASME V V 10 – 2006*.
- Balci, O. (1998). Verification , Validation and Testing. In J. Banks (Ed.), *Handbook of simulation:Principles, methodology, advances, applications, and practice* (Vol. 10, pp. 335-393.). John Wiley & Sons, Inc. <https://doi.org/10.1002/9780470172445.ch10>
- Chollet, F. (2018). Deep Learning with Python. United States: Manning Publications.
- DoD (1994). *DoD Directive Number 5000.59: DoD Modeling and Simulation (M&S) Management*.
- Fayyad, U., Piatetsky-Shapiro, G., & Smyth, P. (1996). The KDD process for extracting useful knowledge from volumes of data. *Communications of the ACM*, 39(11), 27-34.
- IEEE (1984). *IEEE Standard Dictionary of Electrical and Electronics Terms*. ANSI/IEEE Std 100 – 1984, New York.
- Oberkamp, W. L., & Roy, C. J. (2010). *Verification and validation in scientific computing*. Cambridge University Press.
- Robinson, S. (2004). *Simulation: The Practice of Model Development and Use* (First edit). John Wiley & Sons, Ltd. <https://doi.org/10.1057/palgrave.jos.4250031>
- Sargent, R. G. (2013). Verification and validation of simulation models. *Journal of Simulation*, 7, 12–24. <https://doi.org/10.1109/WSC.1998.744907>
- Schlesinger, S. (1979). Terminology for model credibility. *Simulation*, 32(3), 103-104.
- Shmueli, G. (2011). *To Explain or to Predict?* 25(3), 289–310. <https://doi.org/10.1214/10-STS330>
- Tol, A., Diallo, S. Y., Padilla, J. J., & Herencia-Zapana, H. (2013). Reference modelling in support of M&S—foundations and applications. *Journal of Simulation*, 7(2), 69–82. <https://doi.org/10.1057/jos.2013.3>