Validity in (Co-)Simulation

Threats, Opportunities and Languages

Keynote @ MPM4CPS 2022

October 23th, 2022

Joachim Denil

With the help and contribution of many!

University of Antwerp

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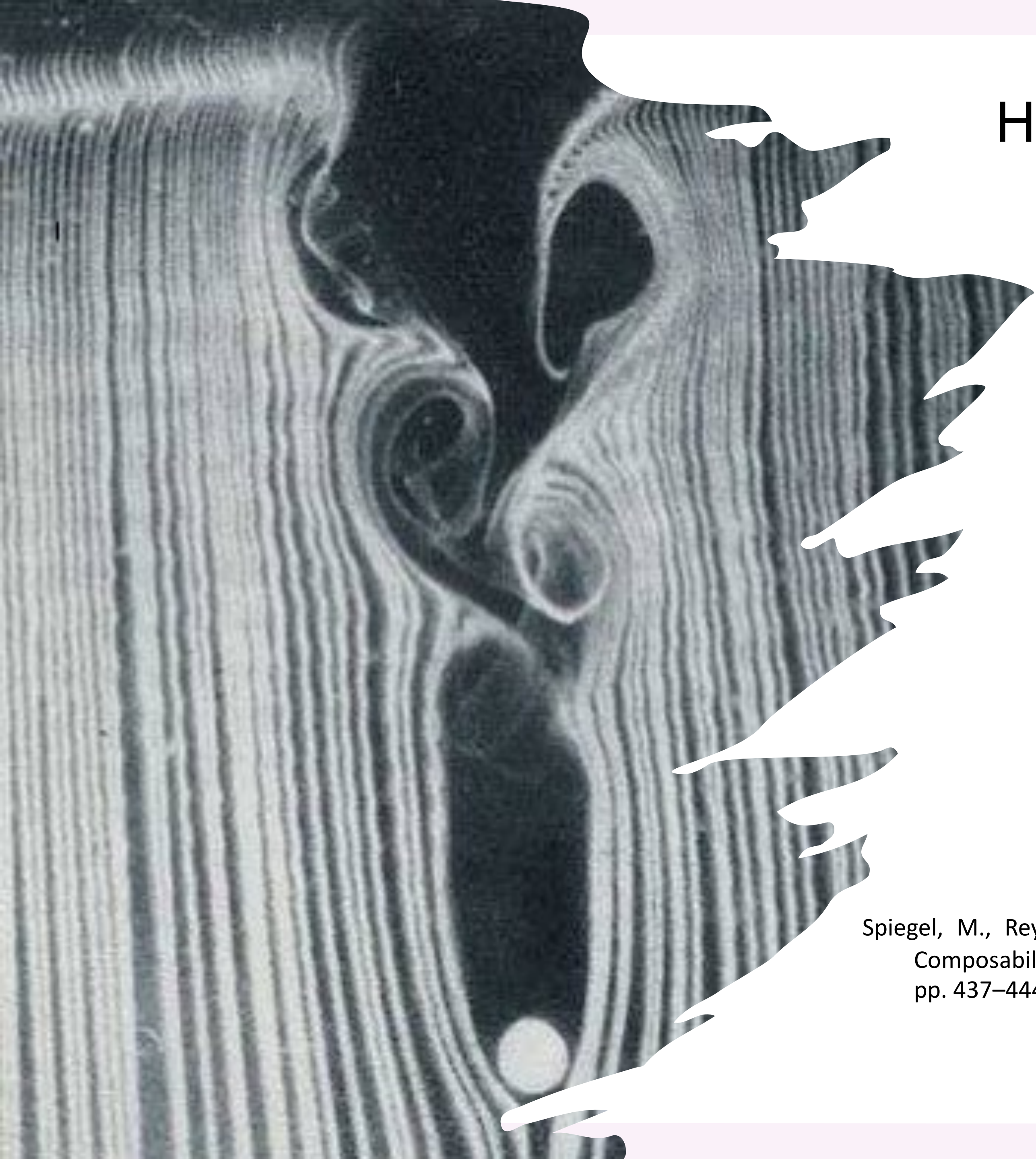
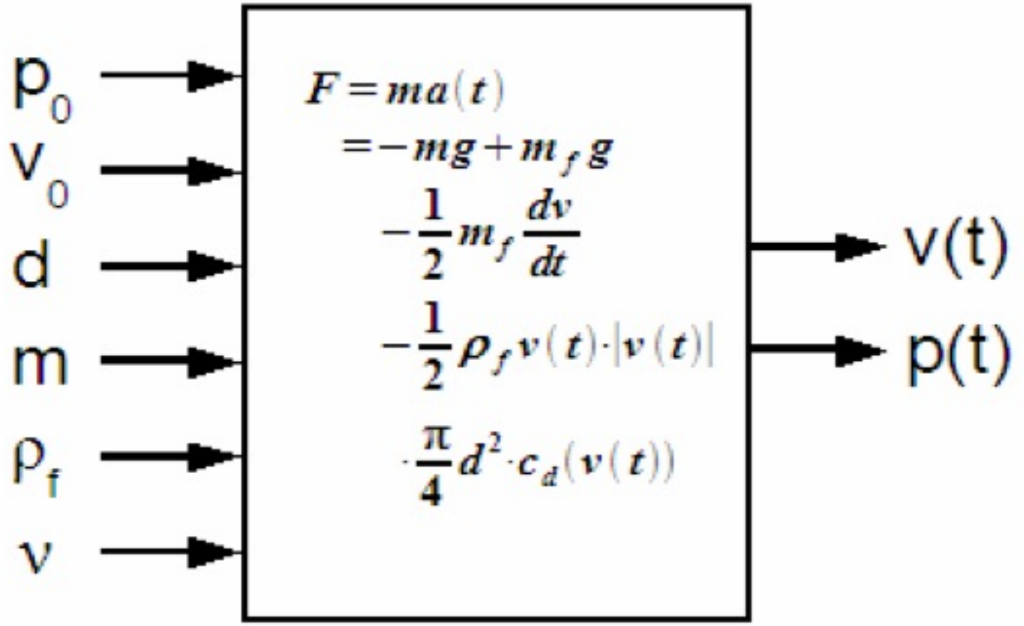


How many contextual constraints can you guess? Under which circumstances can I use this model?



Spiegel, M., Reynolds, P. F., & Brogan, D. C. (2005). A Case Study of Model Context for Simulation Composability and Reusability. In *Proceedings of the Winter Simulation Conference, 2005.* (Vol. 2005, pp. 437–444). IEEE. http://doi.org/10.1109/WSC.2005.1574279

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1. Invariant Constraints

1.a Sphere Attributes

1. Sphere Property - The body is a sphere and it remains spherical.
2. Smooth Property - The body is smooth and it remains smooth.
3. Impermeable Property - The body is completely impermeable.
4. Initial Velocity - The body has an initial velocity of v_0 that has no horizontal component of motion.
5. Angular Velocity - The body has no initial angular velocity.
6. Constant Mass - The mass of the body remains constant over time. The body does not experience ablation or accretion.
7. Constant Diameter - The diameter of the body remains constant over time.
8. Distribution of Mass - The body has a centrally symmetric mass distribution that remains constant over time.
9. Uncertainty Principle - The diameter of the body is much greater than the Plank length.
10. Brownian Motion - The mass and diameter of the body are large enough such that Brownian motion of the fluid has negligible impact on the body.
11. General Relativity - The mass of the body is low enough to ignore the gravitational curvature of space-time.

1.b Fluid Attributes

12. Fluid Density - The fluid density is constant. The fluid is incompressible.
13. Fluid Pressure - The fluid pressure is constant.
14. Fluid Temperature - The fluid temperature is constant.
15. Kinematic Viscosity - The kinematic viscosity is constant. The medium is a Newtonian fluid.
16. Stationary Fluid - The fluid is stationary apart from being disturbed by the falling body.
17. Infinite Fluid - The volume of the fluid is large enough to completely envelope the sphere. The movement of the fluid is not restricted by a container such as a pipe or tube.

1.c Earth Attributes

18. Flat Terrain - The ground does not have terrain and remains flat for all $t > 0$.
19. Coriolis Effect - The Earth is not rotating. We ignore the Coriolis effect.

2. Dynamic Constraints

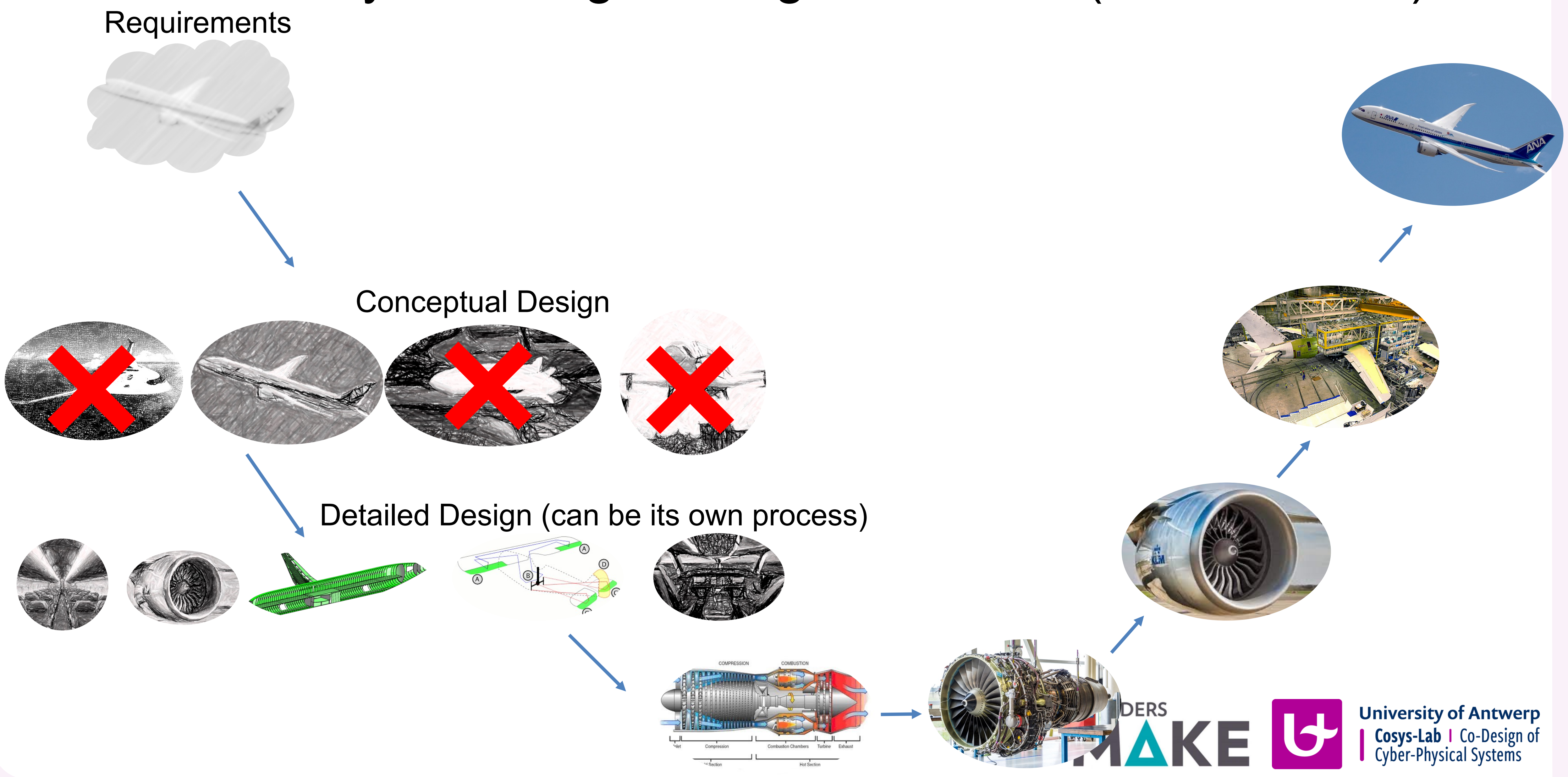
20. Mach Speed - The velocity of the body is sufficiently less than the speed of sound for that medium.
21. Special Relativity - The velocity of the body is sufficiently less than the speed of light for that medium.
22. Reynolds Number - The Reynolds number remains between 10^{-2} and 10^{7} for all $t > 0$. The Reynolds number is a function of velocity.

3. Inter-Object Constraints

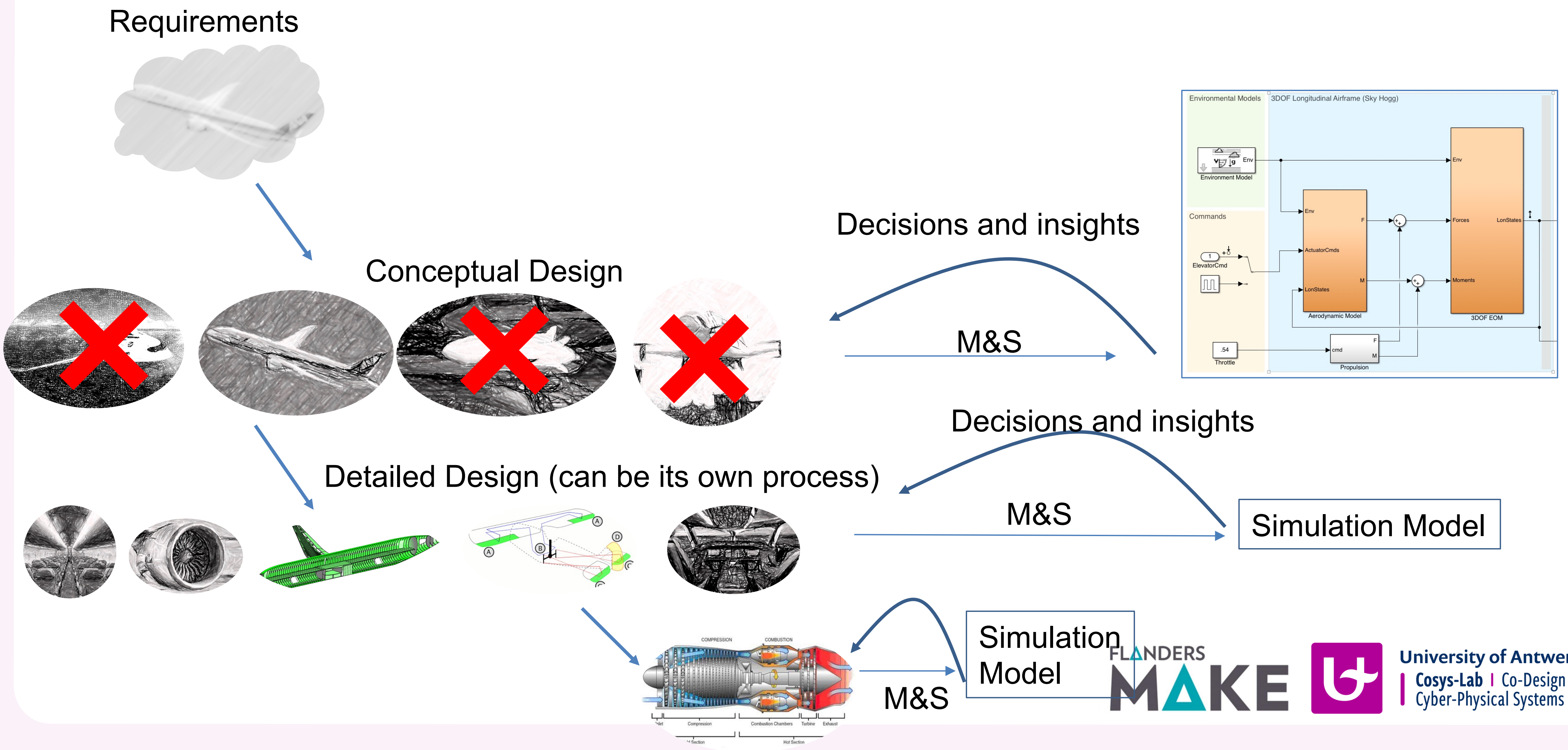
23. Sphere/Fluid Interaction - The body and the fluid interact only through buoyancy and drag. For example, the body cannot dissolve in the fluid, nor can the body transfer heat to the fluid.
24. Sphere/Earth Interaction - The body and the earth interact only through the gravitational force.
25. Fluid/Earth Interaction - The fluid and the earth do not interact.
26. Closed System - The Earth, sphere, and fluid do not interact with any other objects.
27. Simple Gravity - Gravity is a constant downward force of $9.8\ m/s^2$.
28. One-Sided Gravity - The mass of the body is much less than the mass of the Earth. The Earth is not affected by the gravitational pull of the body.
29. Inelastic Collision - The collision between the sphere and the ground is perfectly inelastic.

Spiegel, M., Reynolds, P. F., & Brogan, D. C. (2005). A Case Study of Model Context for Simulation Composability and Reusability. In *Proceedings of the Winter Simulation Conference, 2005.* (Vol. 2005, pp. 437–444). IEEE. http://doi.org/10.1109/WSC.2005.1574279

Model-Based System Engineering Processes (architectures)



Simulation @ Dev



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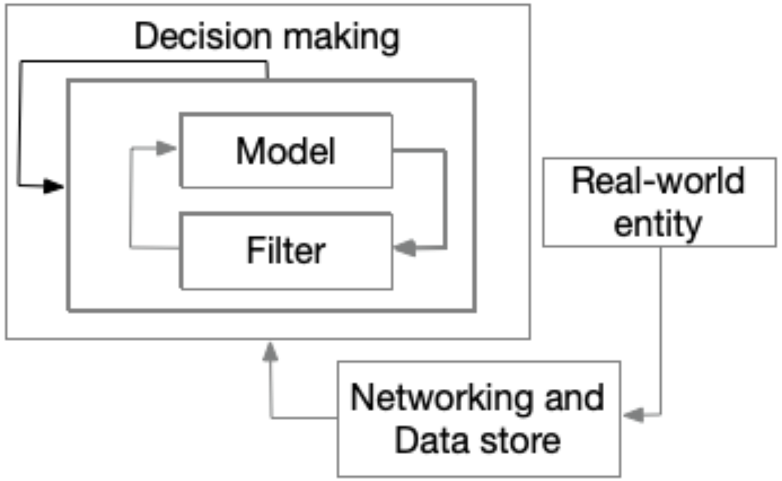
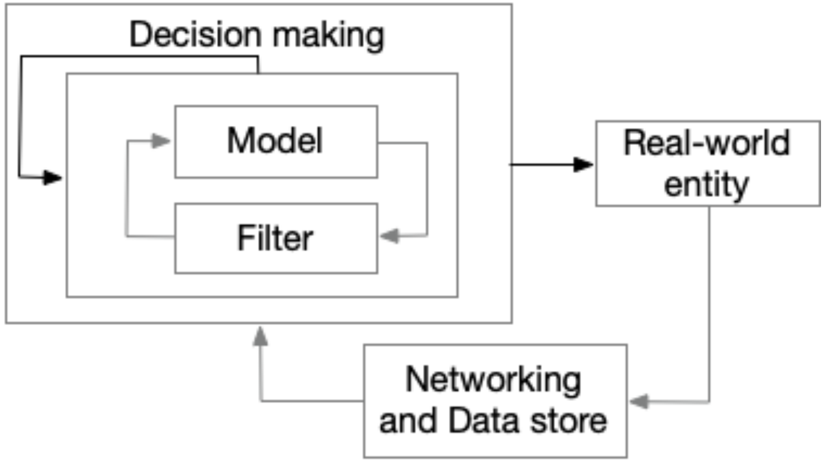
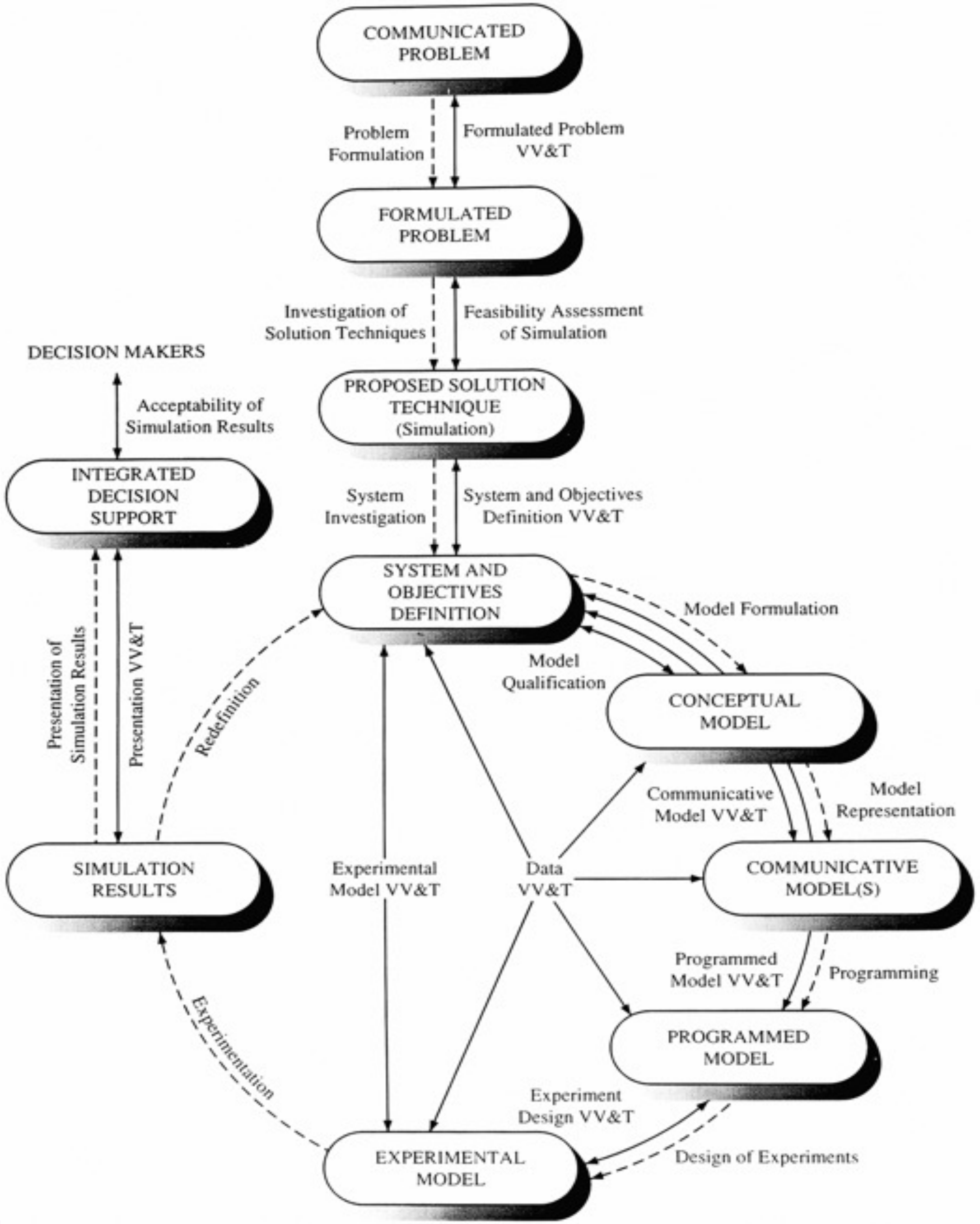
Simulation @ Ops

Digital Shadow



Digital Twin

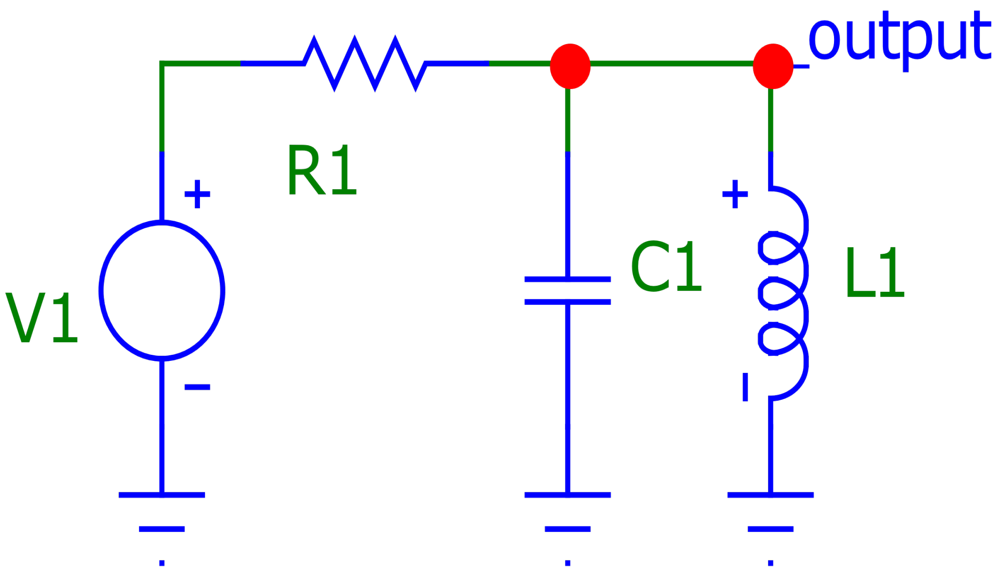


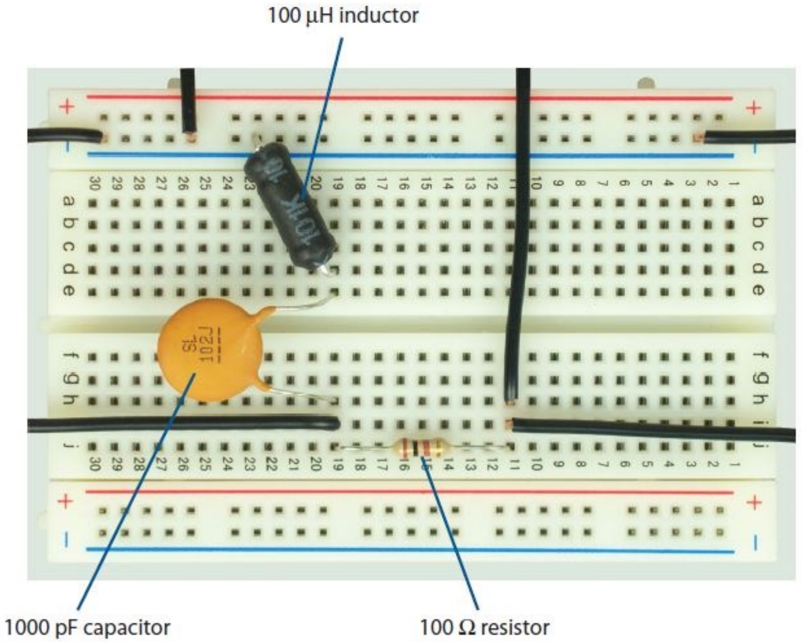


Simulation Workflow

Balci, Osman. "Validation, verification, and testing techniques throughout the life cycle of a simulation study." *Annals of operations research* 53.1 (1994): 121-173.

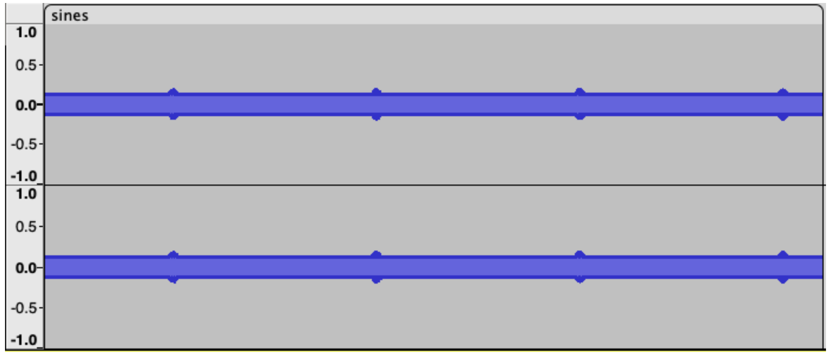
Running Example: Notch Filter

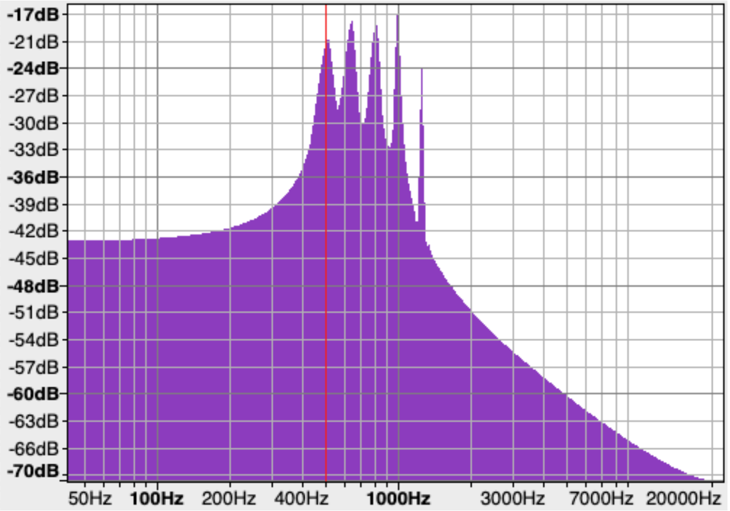


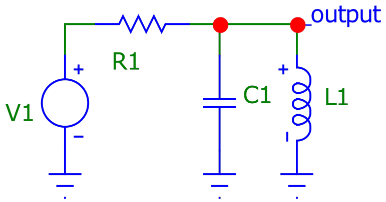


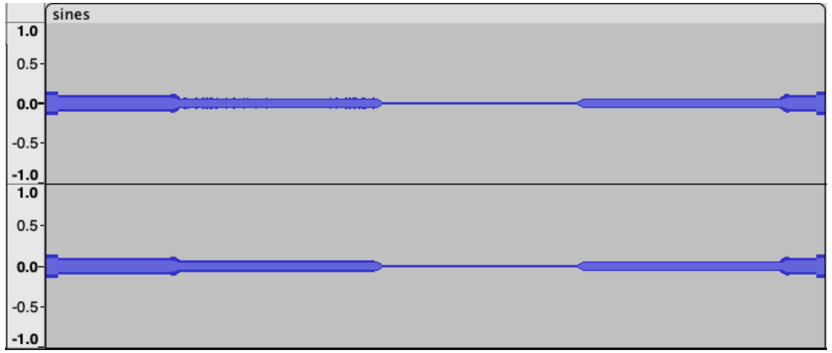
From: Mertens, Joost, and Joachim Denil. "ESS: EMF-Based Simulation Specification, A Domain-Specific Language For Model Validation Experiments." *2022 Annual Modeling and Simulation Conference (ANNSIM)*. IEEE, 2022.

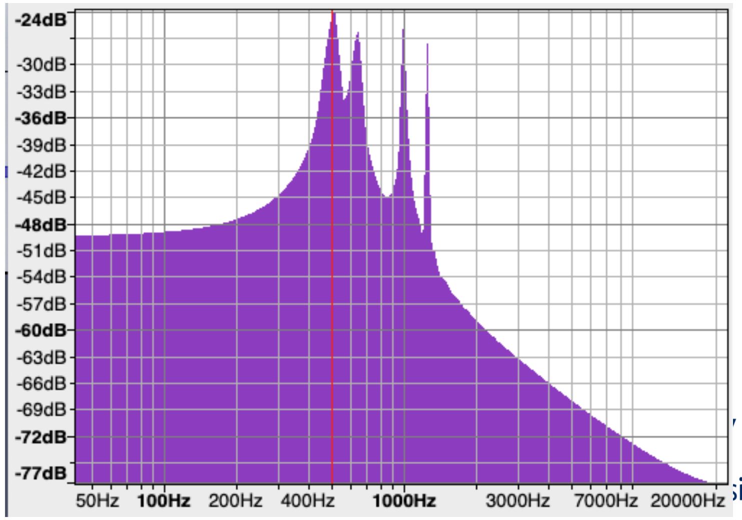
Running Example: Notch Filter





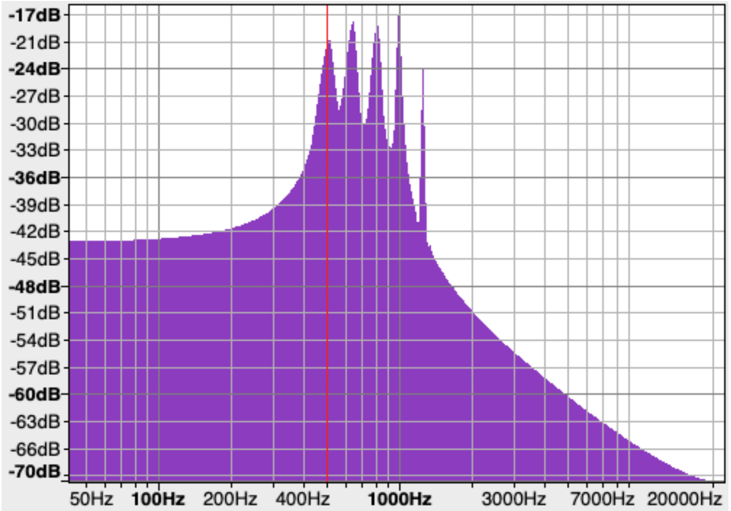




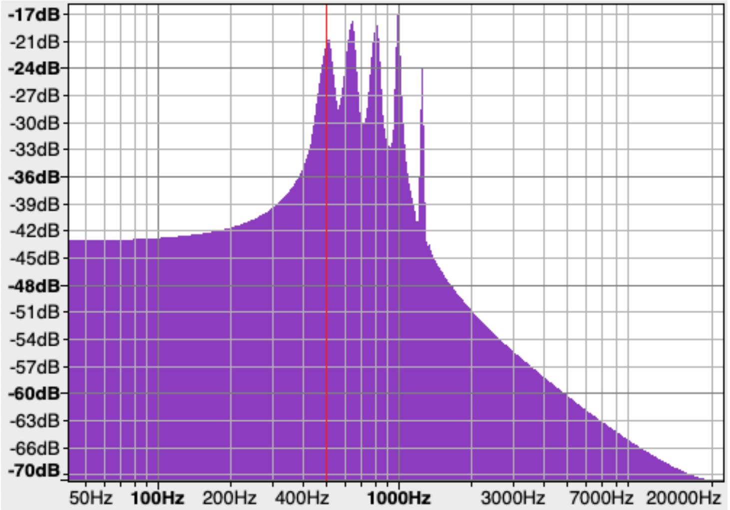


Properties of Interest (PoI)

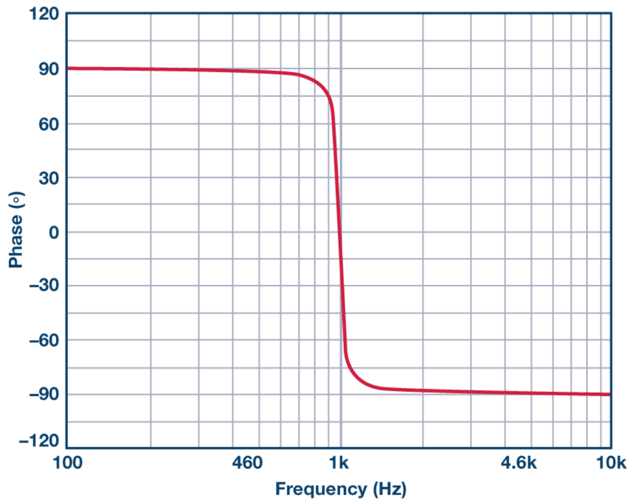
What property are you interested in?



Quality Factor?



Rejection Frequency?



Phase Shift?

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Difficulty to Predict and/or Measure PoI

x = dependent variable

$\int(\int(\int x\,dx)\,dx)\,dx$ $\quad \int(\int x\,dx)\,dx$ $\quad \int x\,dx$ $\quad x$ $\quad \frac{dx}{dt}$ $\quad \frac{d^2x}{dt^2}$ $\quad \frac{d^3x}{dt^3}$

less difficult — more difficult

From: Oberkampf and Roy, Verification and Validation in Scientific Computing, Cambridge, 2010

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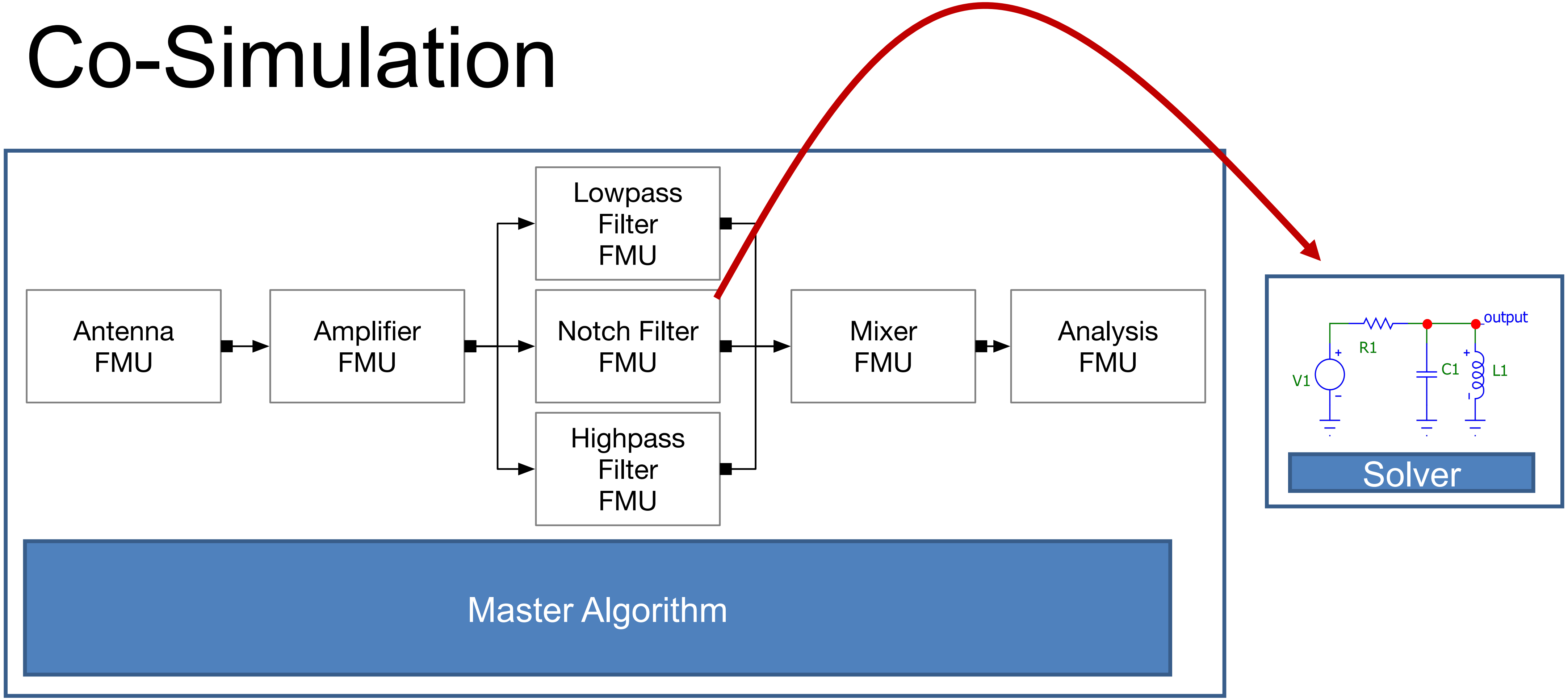
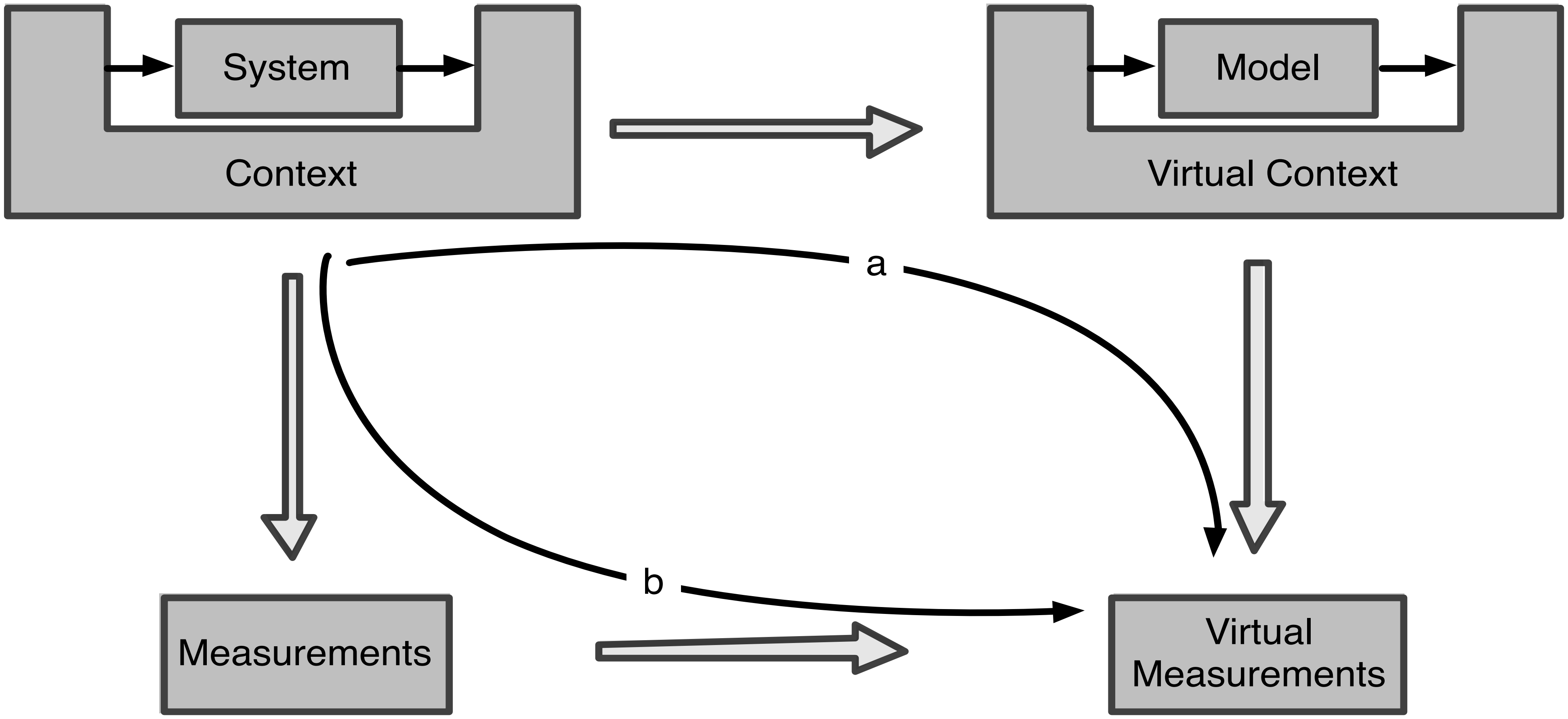
Co-Simulation



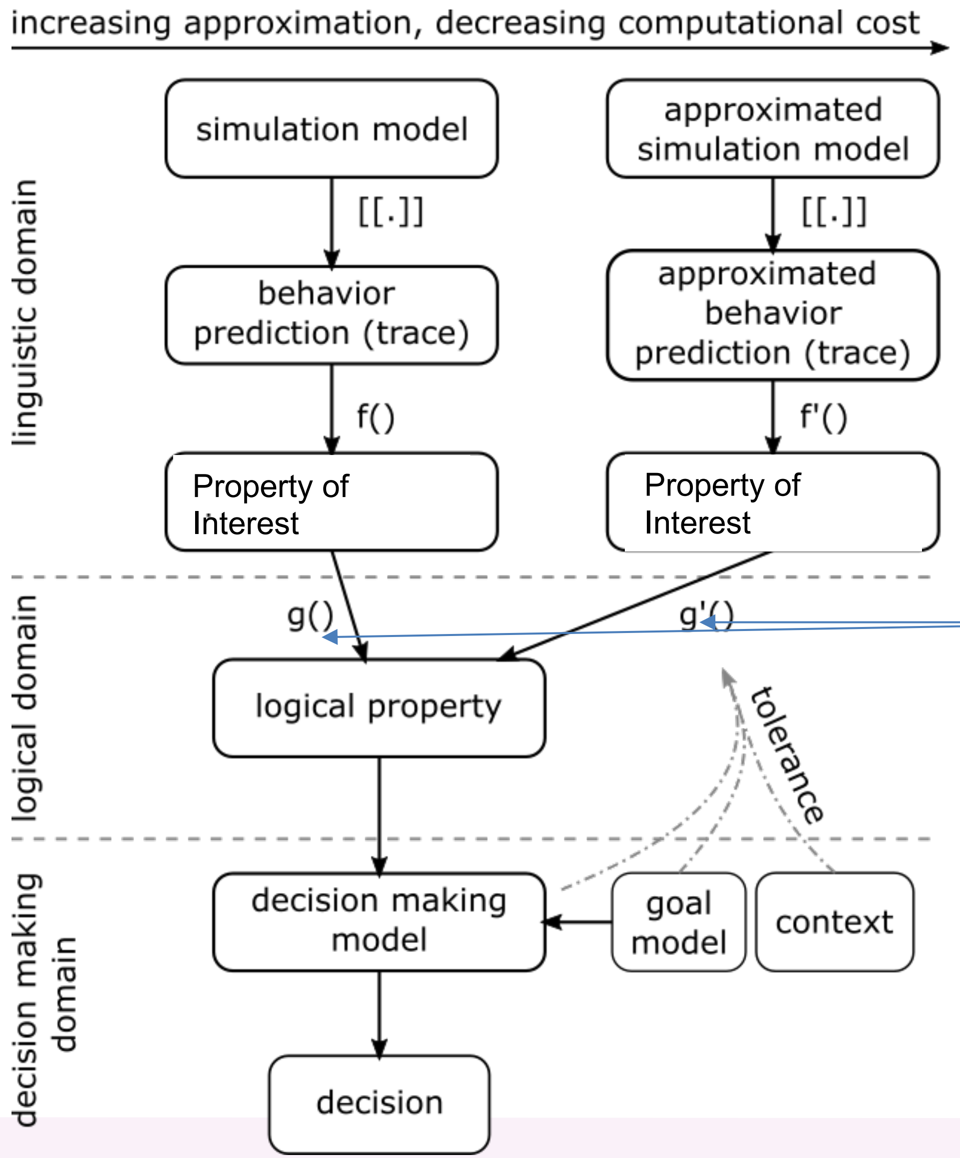
What is Validity?

"A computerized model within its domain of applicability possesses a satisfactory range of accuracy consistent with the intended application of the model" Schlesinger et al. 1979 (SCS Working group)

Substitutability

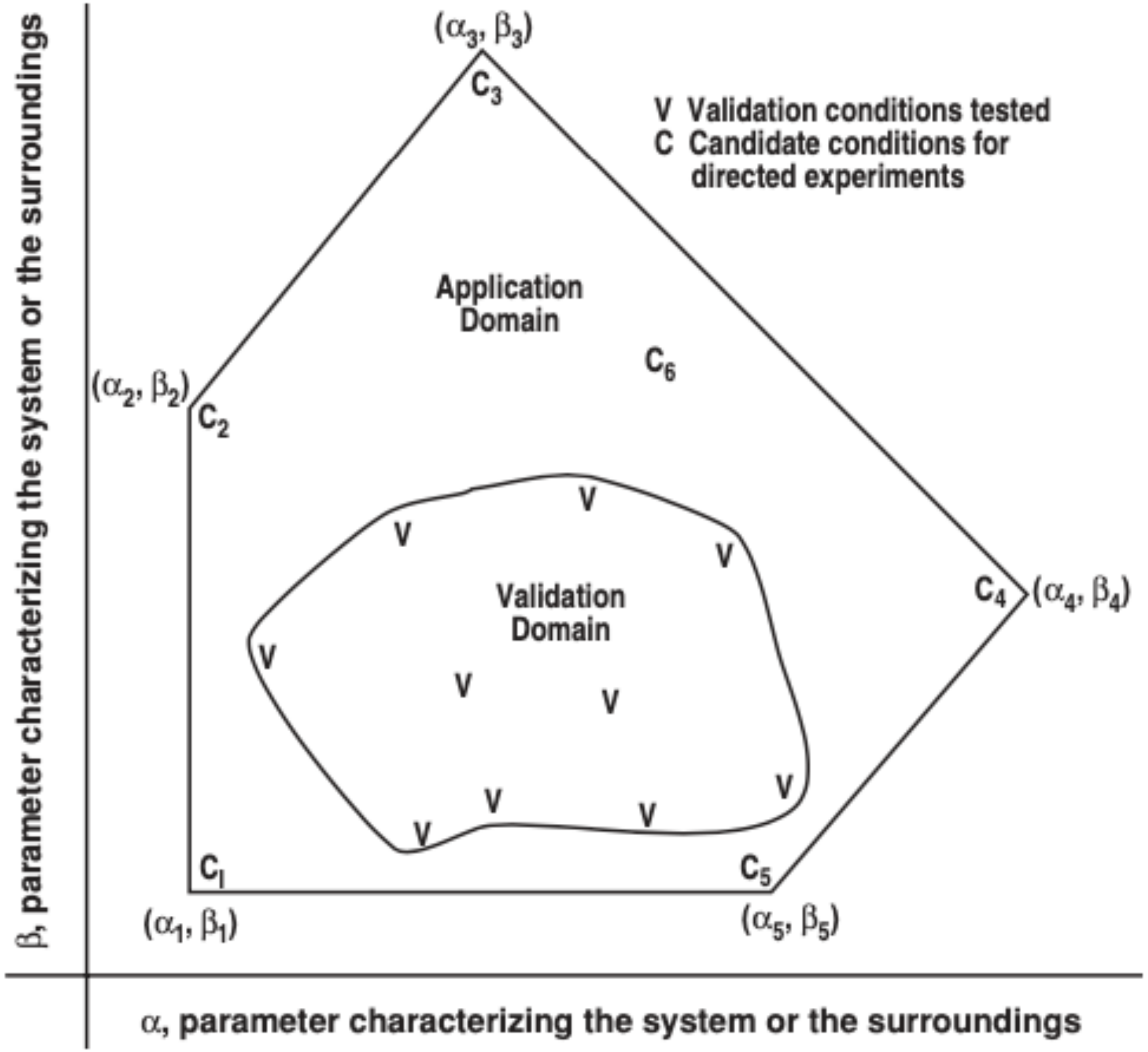


The same applies for Models of Models



'Distance'

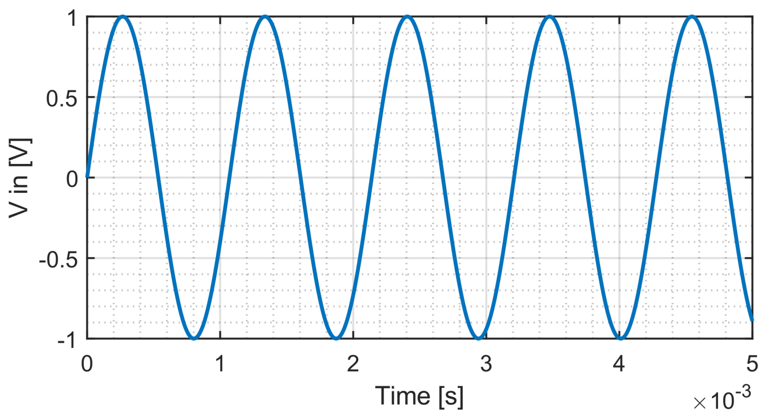
Based on requirements

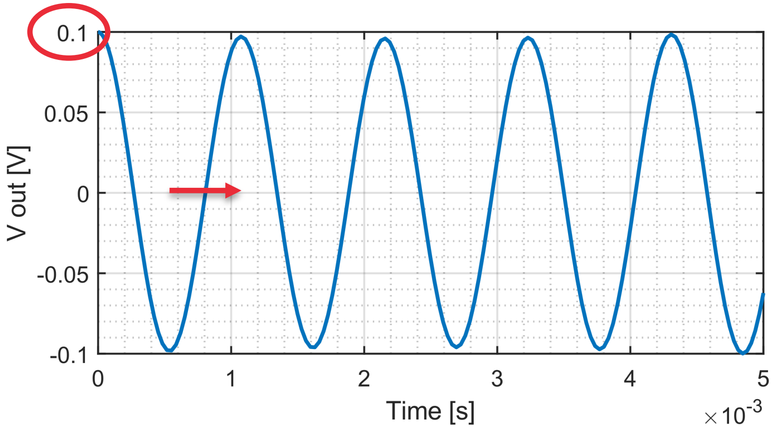


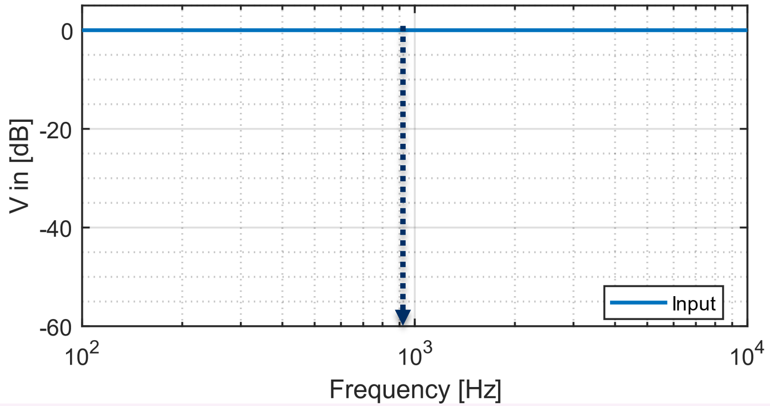
Valid where?

From: Oberkampf and Roy, Verification and Validation in Scientific Computing, Cambridge, 20

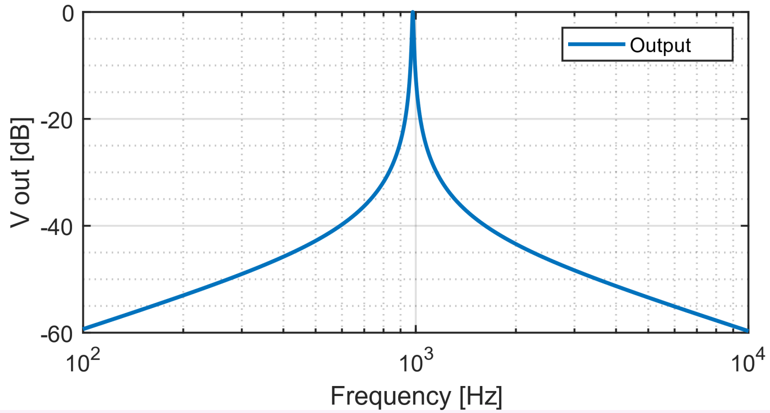
Face Validity: Distance to the Mental Model of Experts



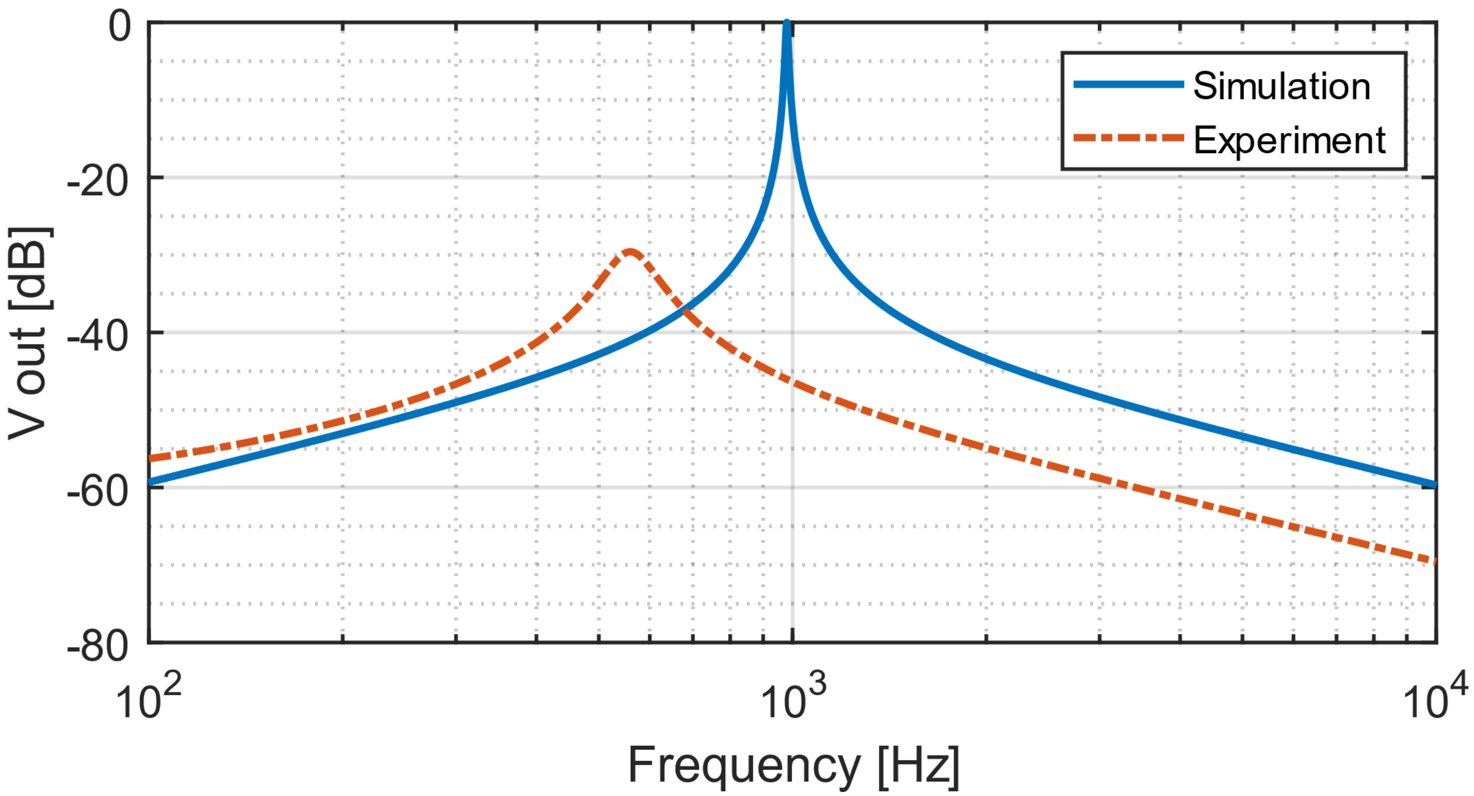




After repeated evaluation at different frequencies, e.g., by performing AC analysis of circuit



How to perform this validation?



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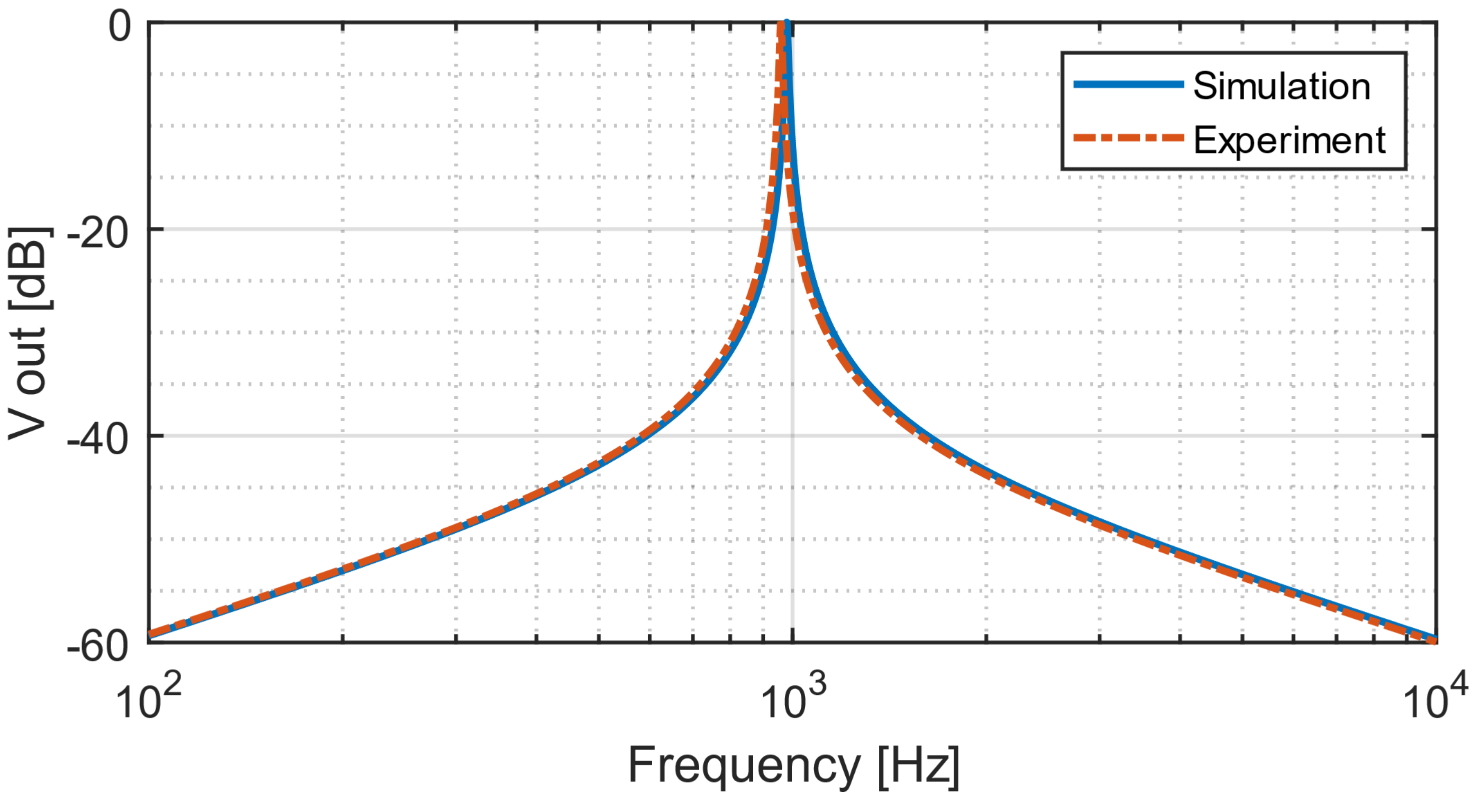

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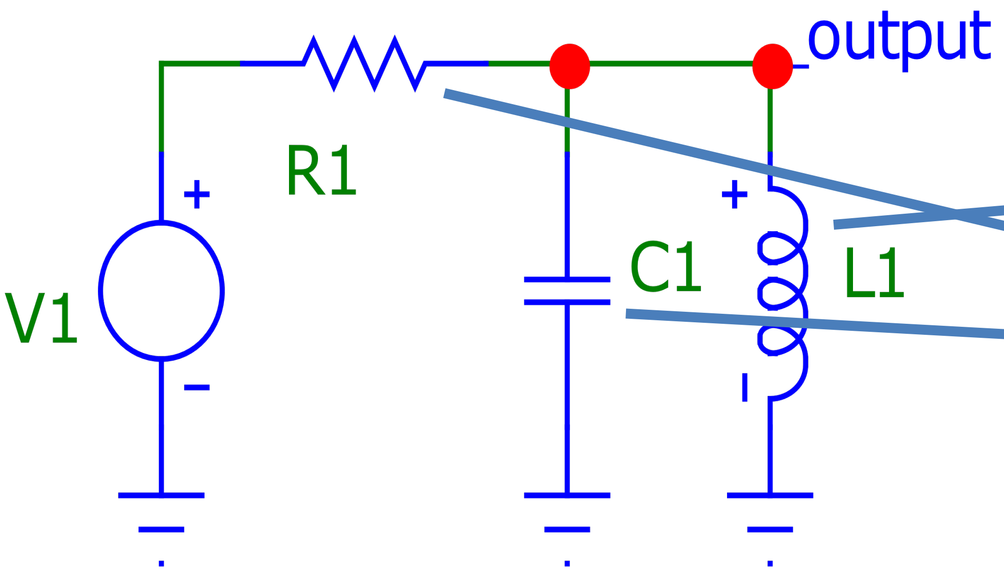
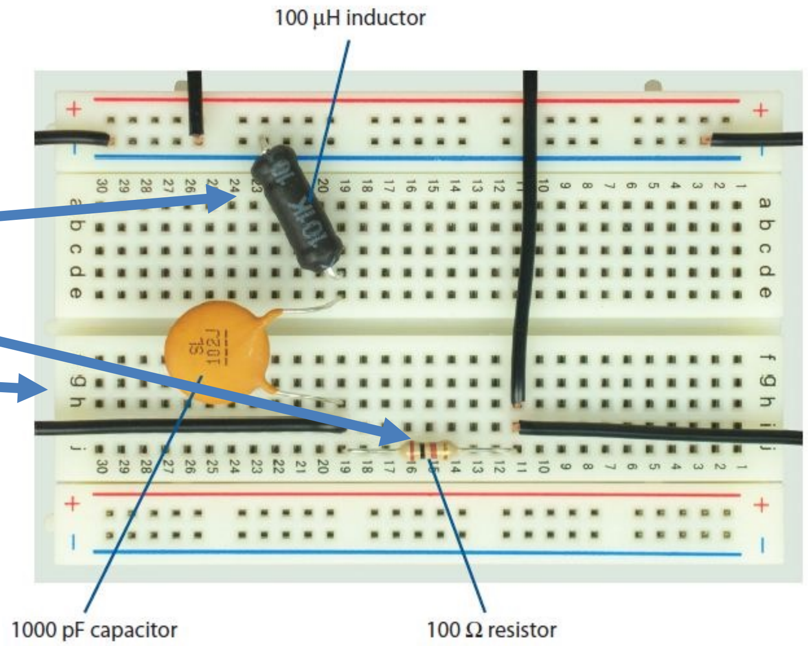
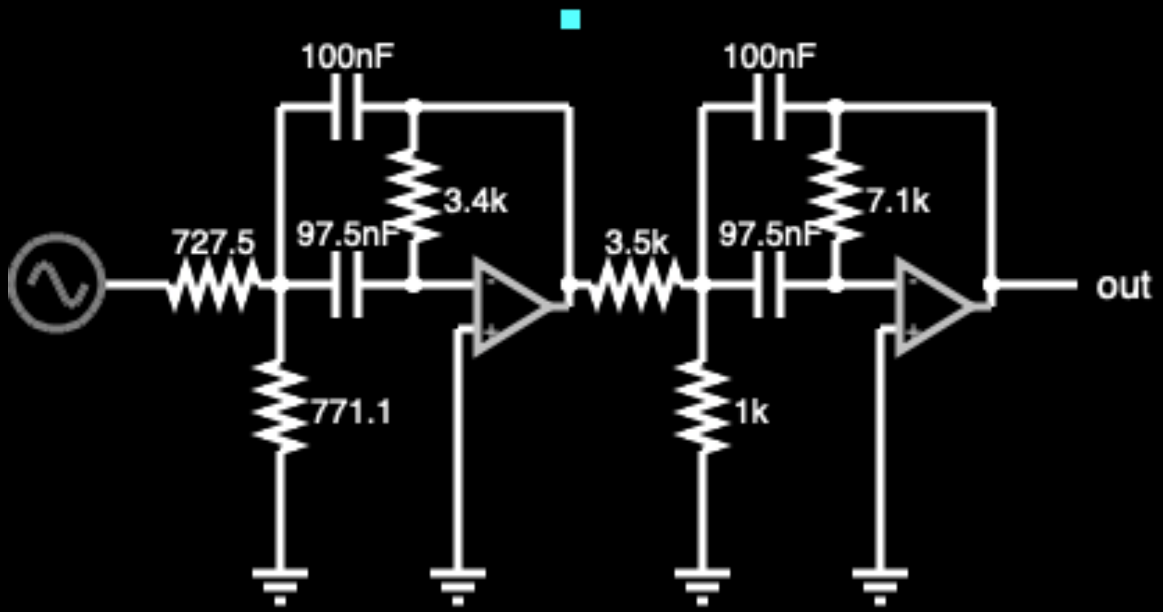
Structural Validity: Distance between Structure of Model and Reality



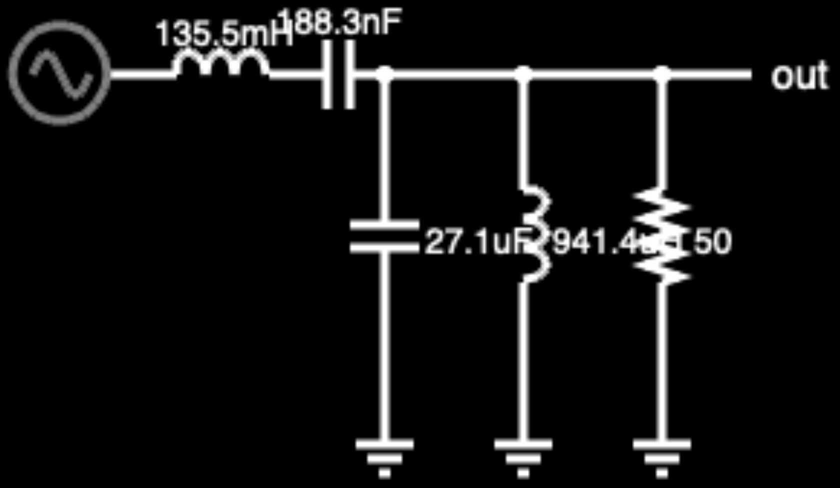


I am I generating the correct behaviour because of the right reasons?

Other Filters Generate the Same Behaviour…



Butterworth filter (active)



Butterworth filter 2nd order (passive)

Generated on: Falstad.com

System's Dynamics

- Structure Verification Test
- Parameter Verification Test
- Extreme Condition Test
- Structure Boundary Adequacy
- Dimensional Consistency

TESTS FOR BUILDING CONFIDENCE IN

SYSTEM DYNAMICS MODELS

Jay W. Forrester

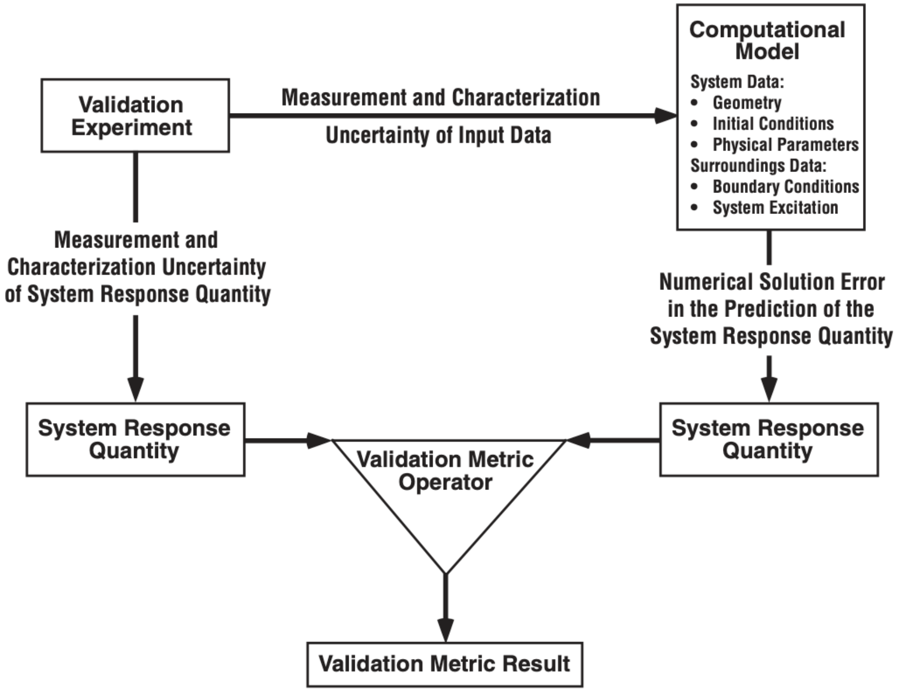
Peter M. Senge

June 8, 1979

System Dynamics Group
Alfred P. Sloan School of Management
Massachusetts Institute of Technology
Cambridge, Massachusetts

Statistical Validity: Statistical Distance between Model and Real-world Results

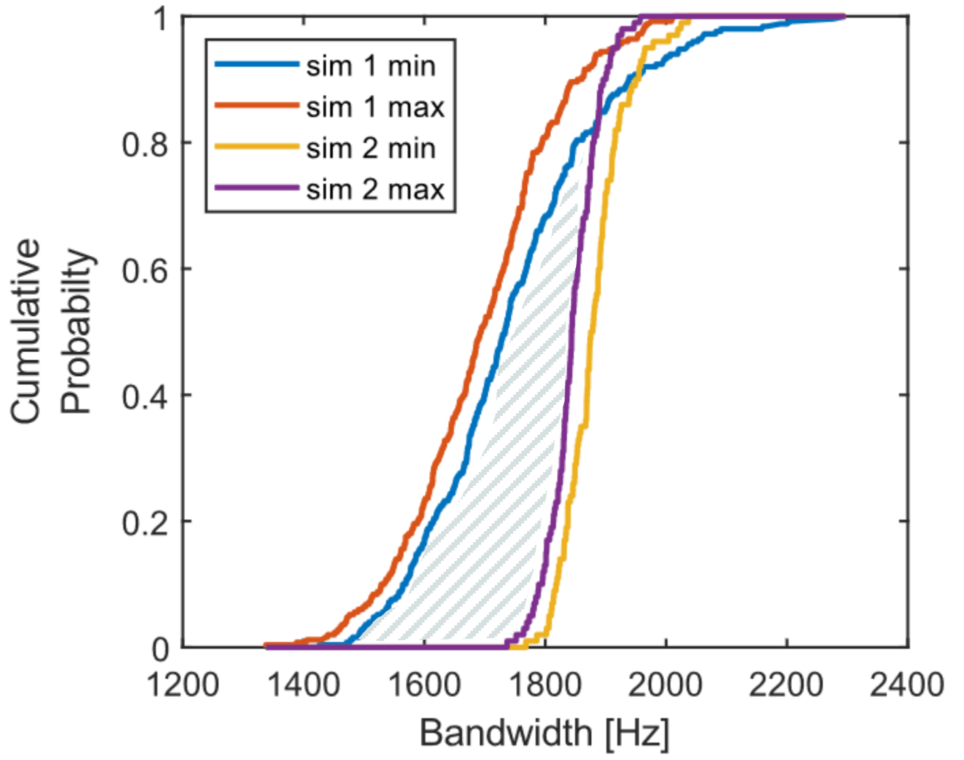
Bayesian – Hypothesis testing – Area metrics



From: Oberkampf and Roy, Verification and Validation in Scientific Computing, Cambridge

Example: CDF Area Metric

- Cumulative Distribution Function (CDF) of *Property of Interest*
- Defined as area enclosed by CDF's
  - Of virtual and real experiment
  - Of two virtual or two real experiments
- Handles any type of uncertainty!
- Unit of area = unit of x-axis
  - Interpretation needs domain knowledge



From: Mertens, Denil,

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Related Concepts (1)

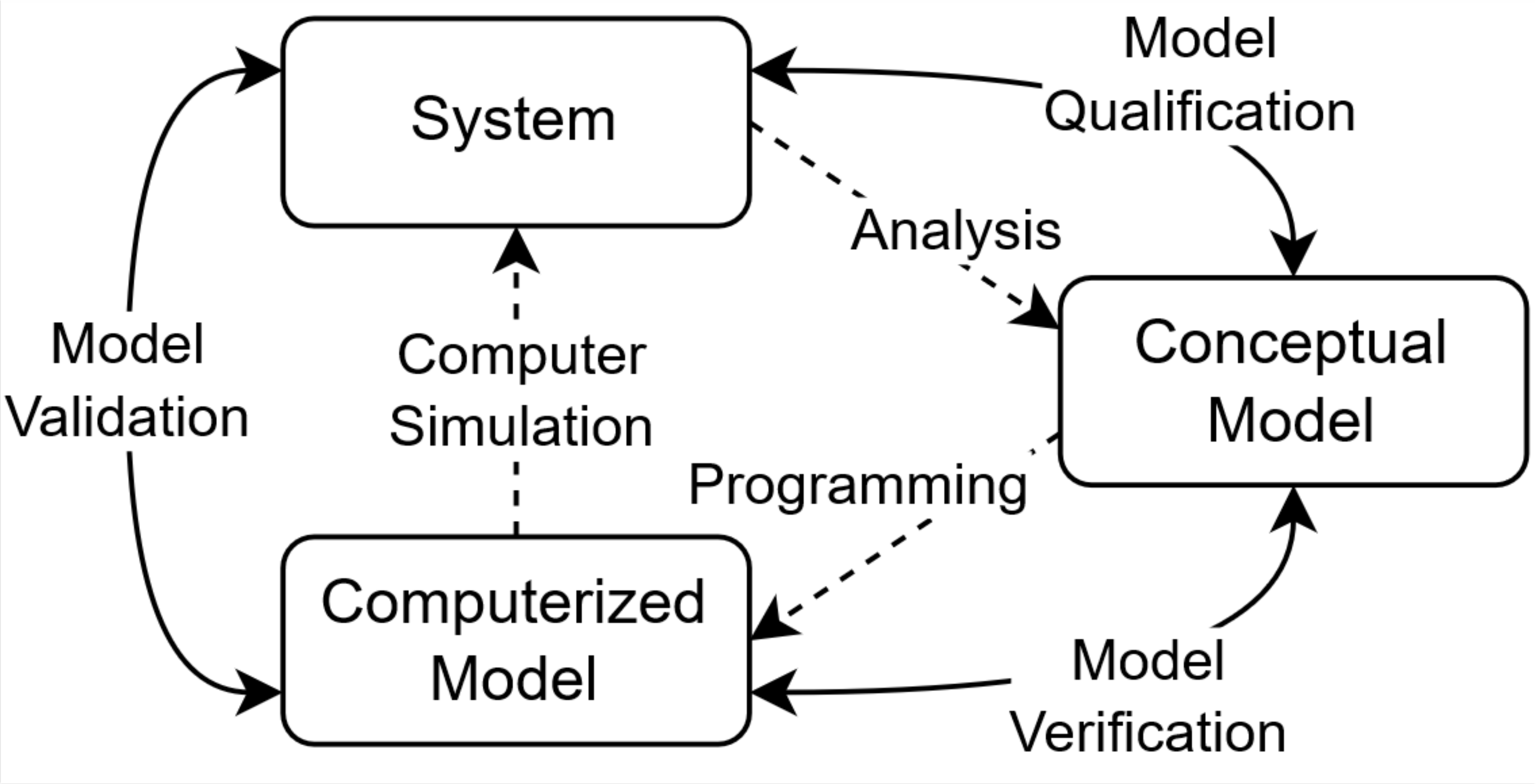


Figure adapted from [1] Schlessingner, S., et al. "Terminology for model credibility" (1979)

Credibility

Is about the *Believability* of a model / Reputation / Trust

Is a broader concept than the validity of a model

Both workflow and artifact

In the eye of the beholder

Example:

Who authored the model?

How did you come up with the model?

How did the model evolve?

Validation activities?

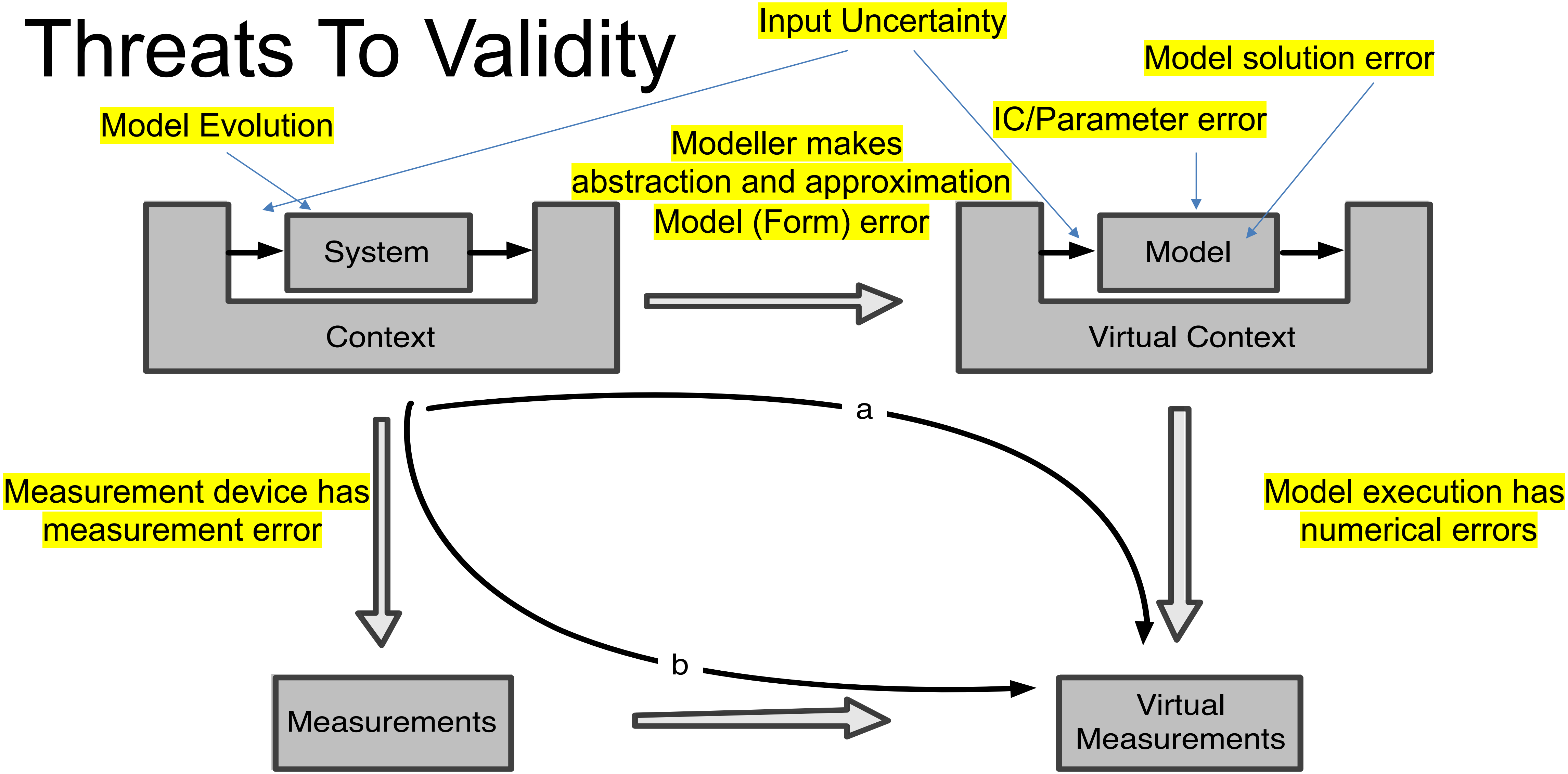
Related Concepts (2)

- Accuracy / Numerical Accuracy
- Precision
- Fidelity (incl. high fidelty, low fidelity)
- Model Prediction
- Calibration
- Tolerance / Robustness
- Uncertainty

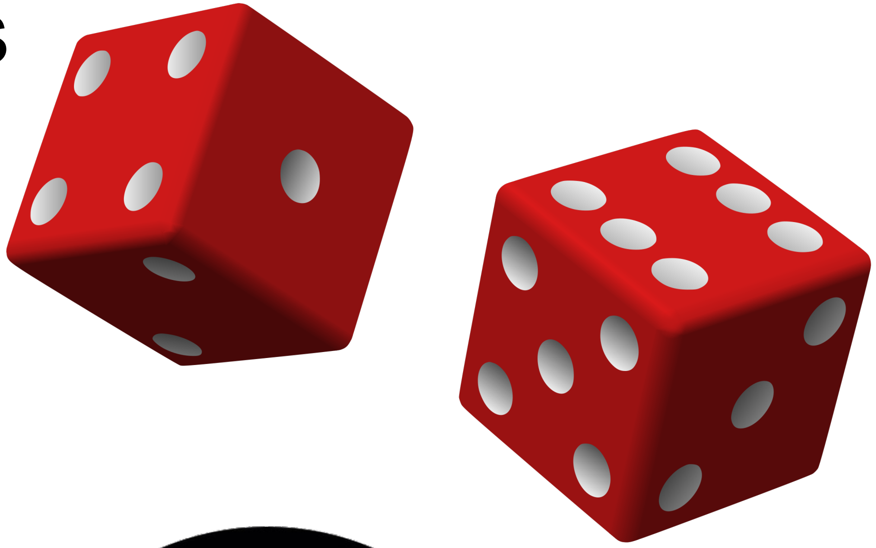
Science vs. Engineering

From: NASA (CC2)

Threats To Validity

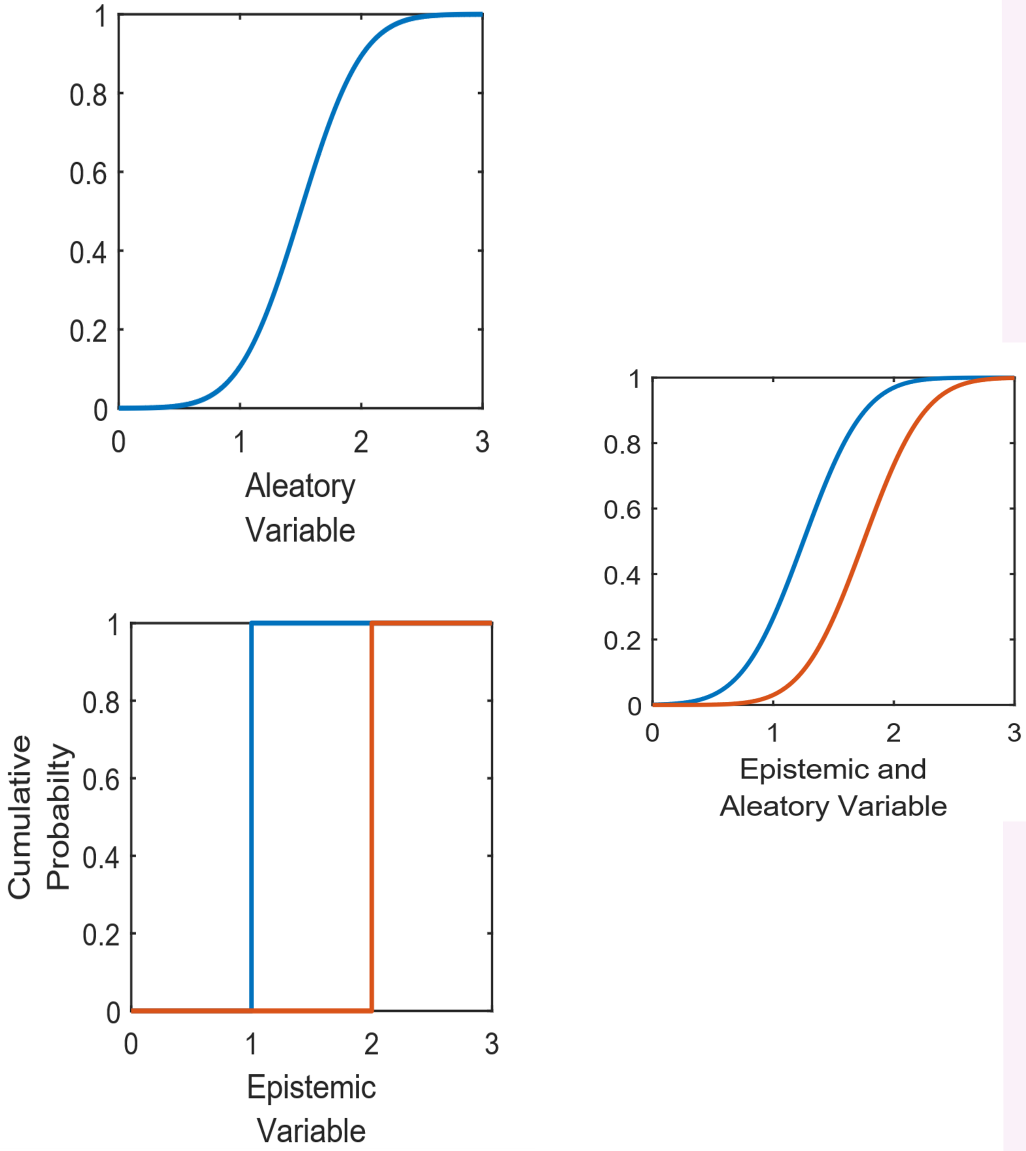


Uncertainties



- Aleatoric

- Epistemic



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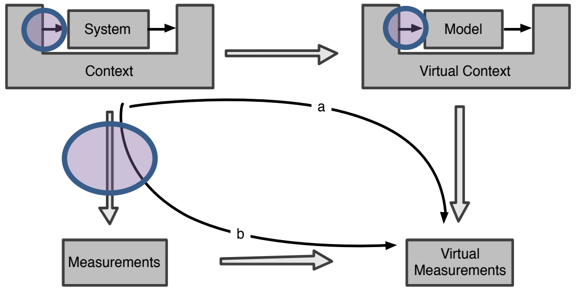
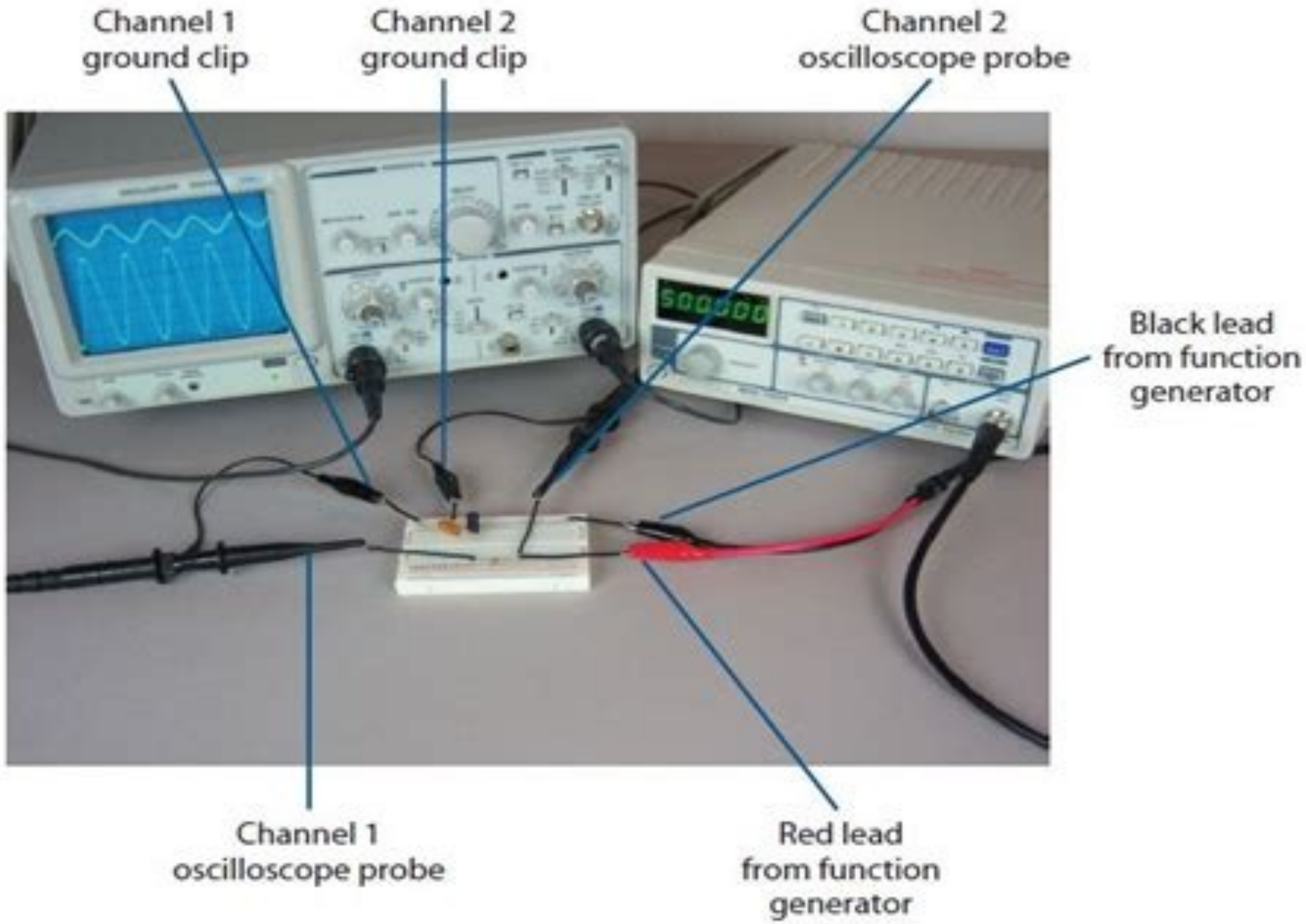
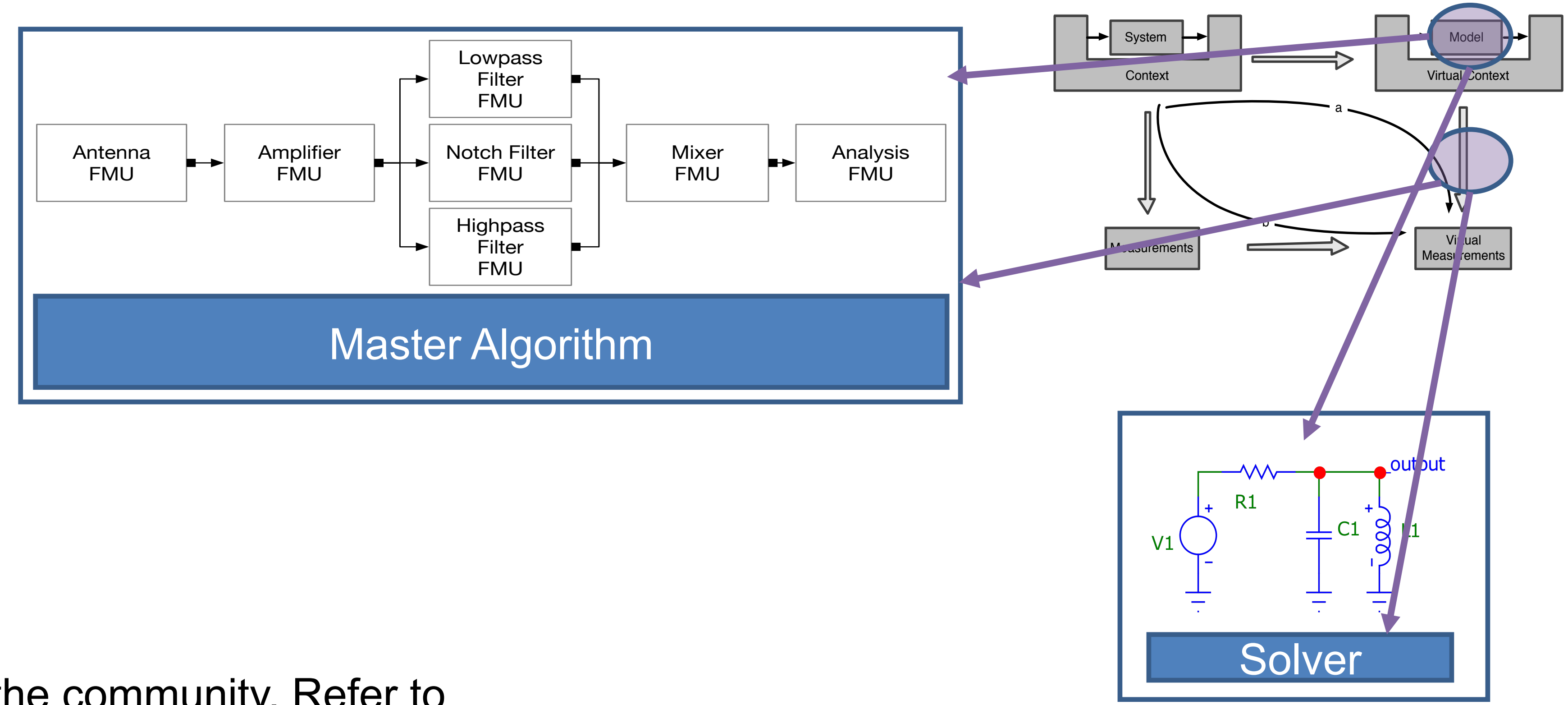
Experiments





Design Of Experiments (both computational as in real-world)

Each Model and Sub-Model needs Verification



Lots of contributions done by the community. Refer to

Gomes C, Thule C, Broman D, Larsen PG, Vangheluwe H. Co-simulation: a survey. ACM Computing Surveys. 2018\

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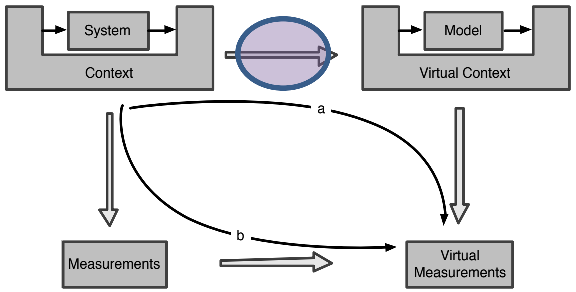
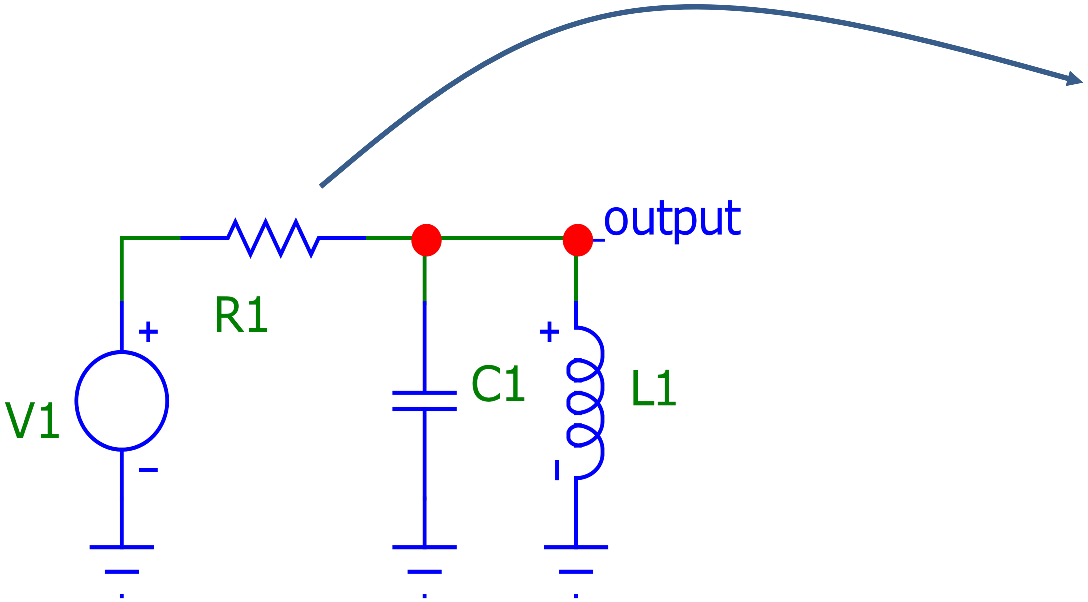
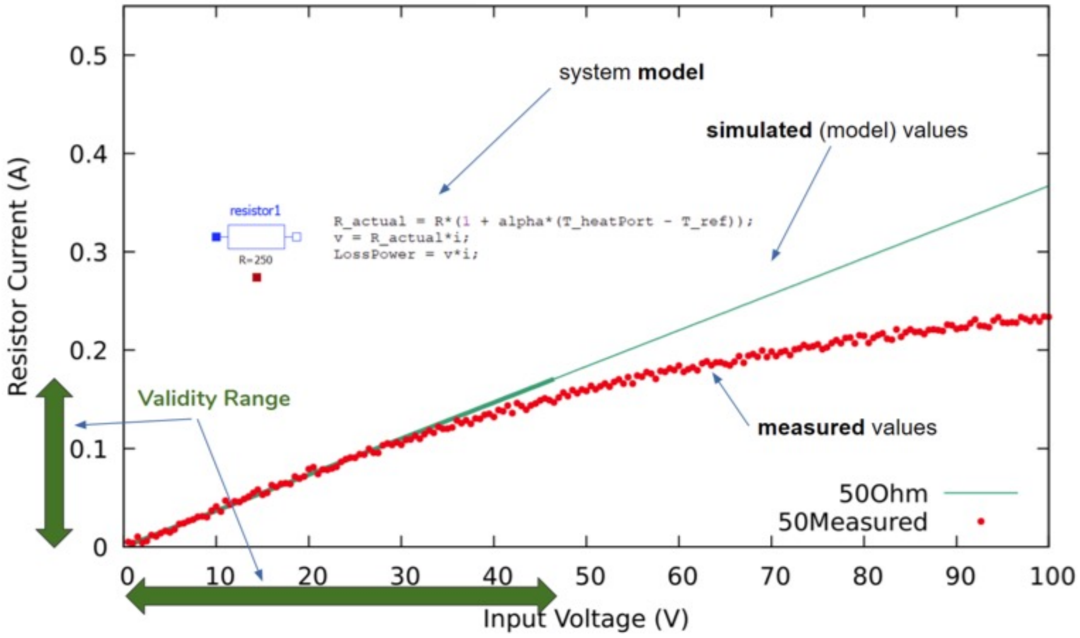
Internal Validity



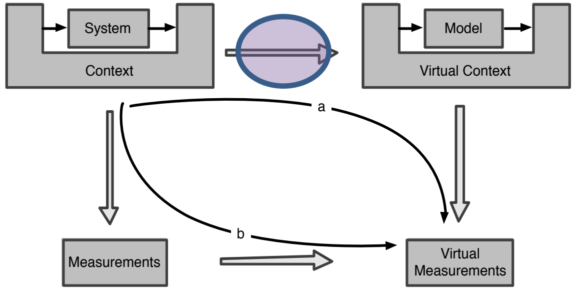




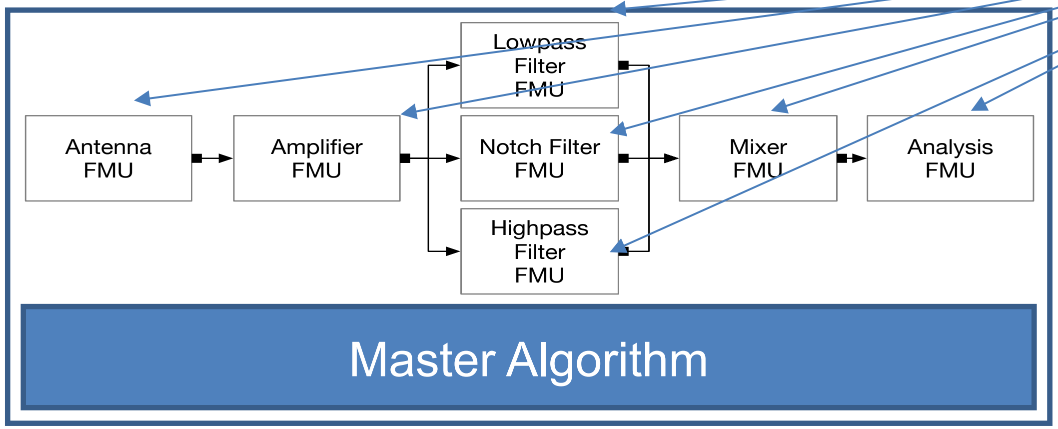
From: Van Mierlo et al. “Exploring Validity Frames in Practice”,

Ohm’s Law (simple form) does not take temperature effect into account

External Composition

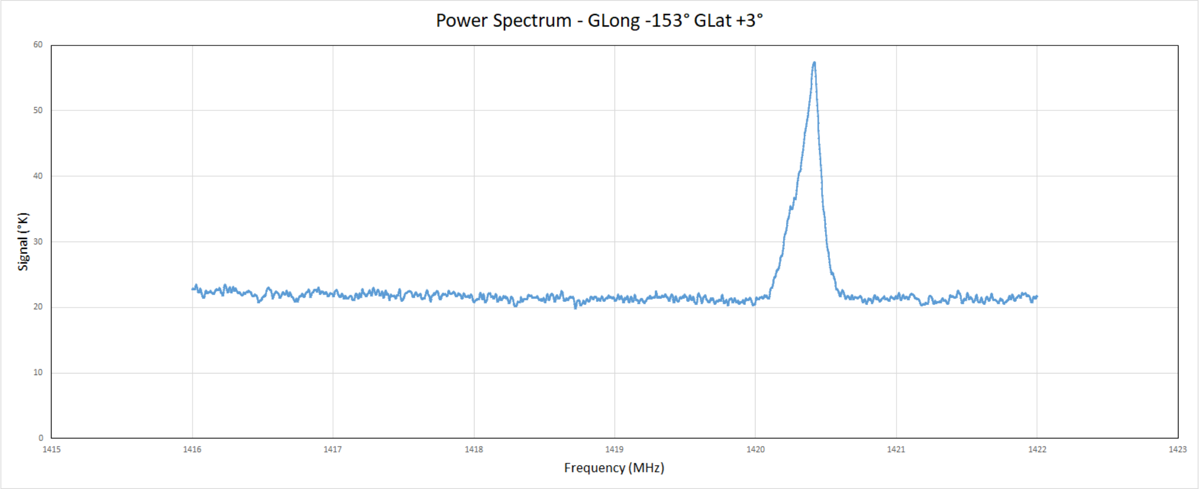


All valid models!



Is the composition valid?

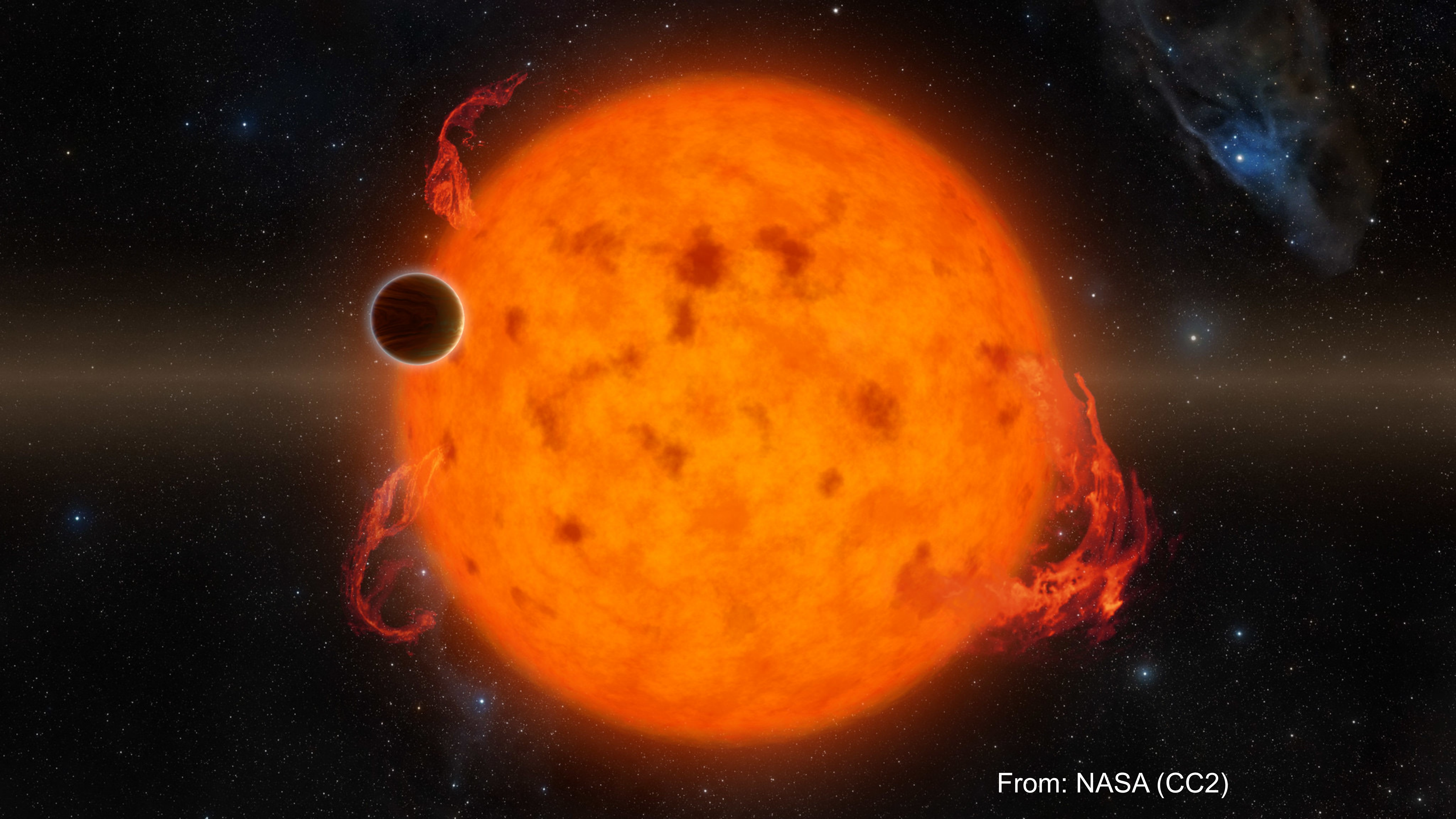
Depends on the PoI!



From: Physics Open-Lab

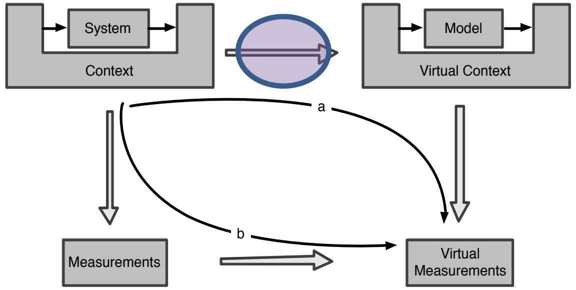
Techniques exist to efficiently propogate through networks

Opportunity: Sensitivity Analysis



From: NASA (CC2)

External Composition



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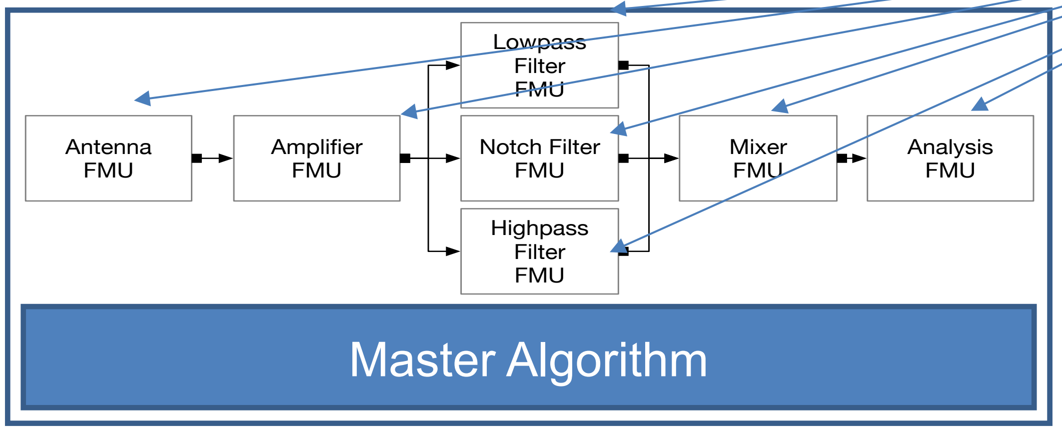

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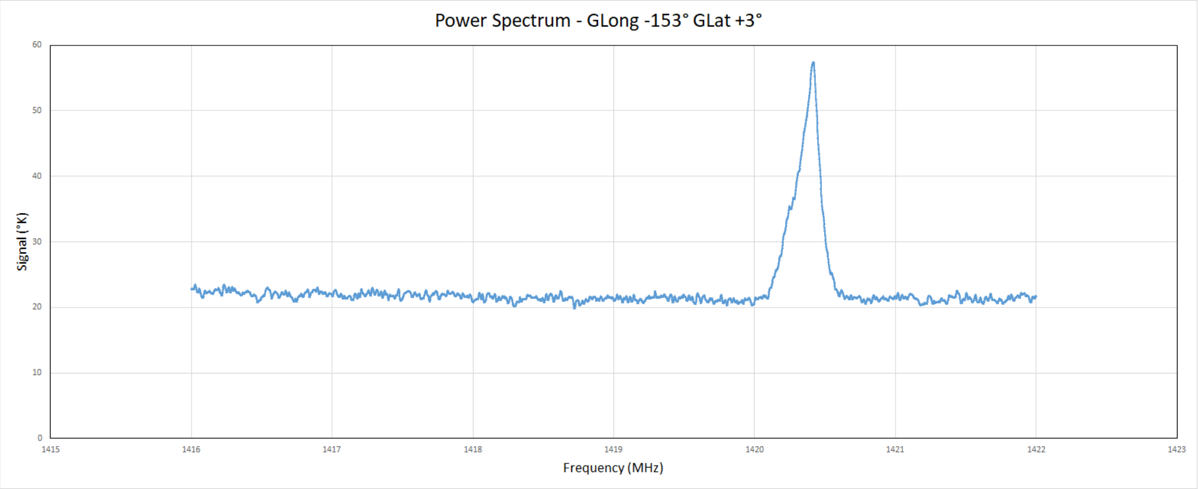
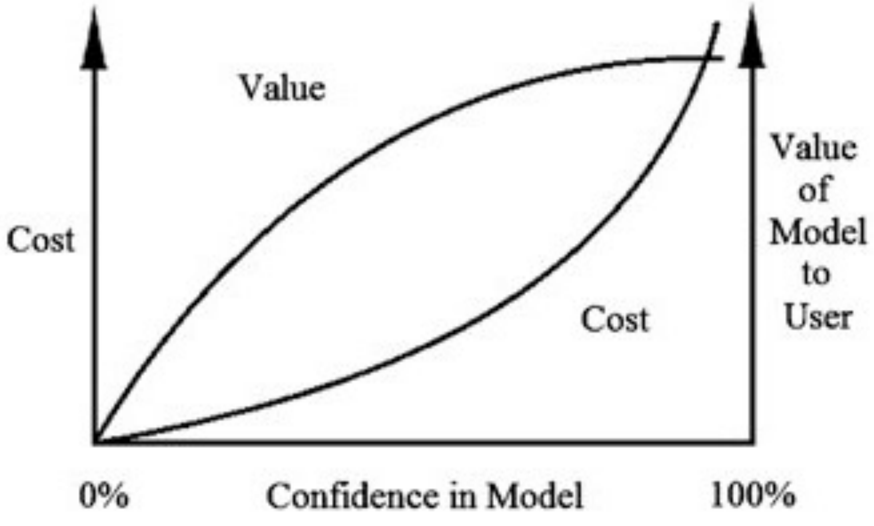


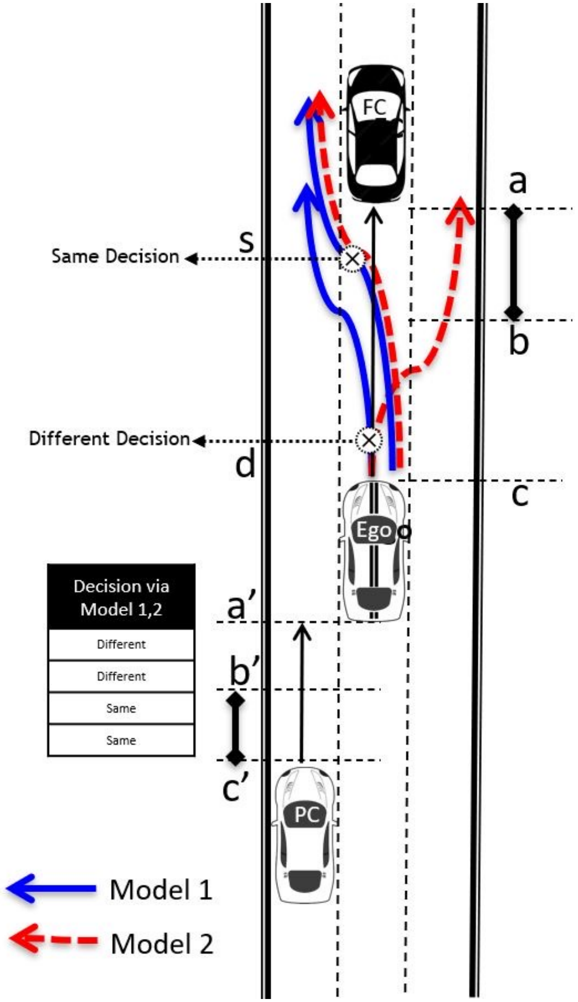
From: Physics Open-Lab

Opportunities: Value and Tolerance

- Uncertainty is not necessarly bad
- Very much related to the goals of the model
- Example: Adaptive Cruise Control Trajectory Prediction (online)



From: Sargent, Verification and validation of simulation models, Journal of Simulation, 2013



From Biglari, Denil, “Model Validity and Tolerance Quantification for Real-time Adaptive Approximation”, MODELS companion, 2022

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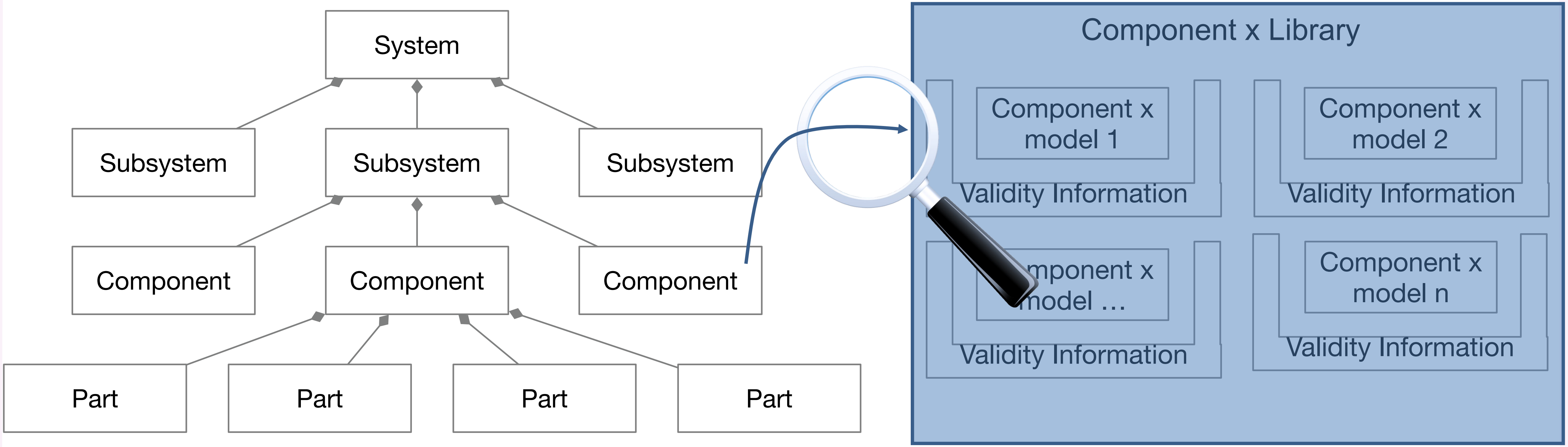
Opportunities: Libraries of Models with Validity Information



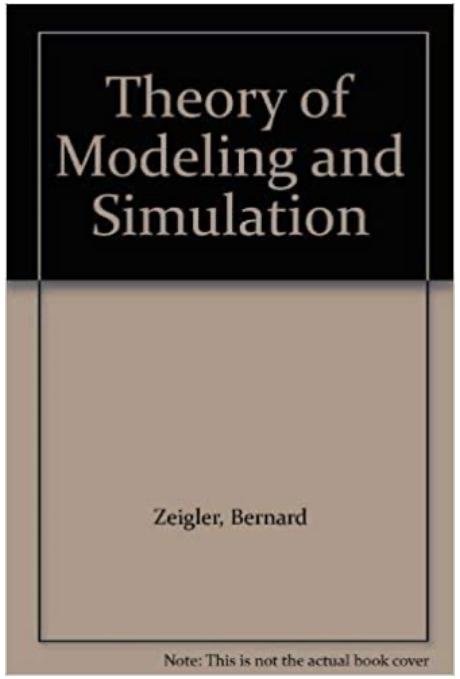
Use the natural hierarchy!

Tool Support for Validity

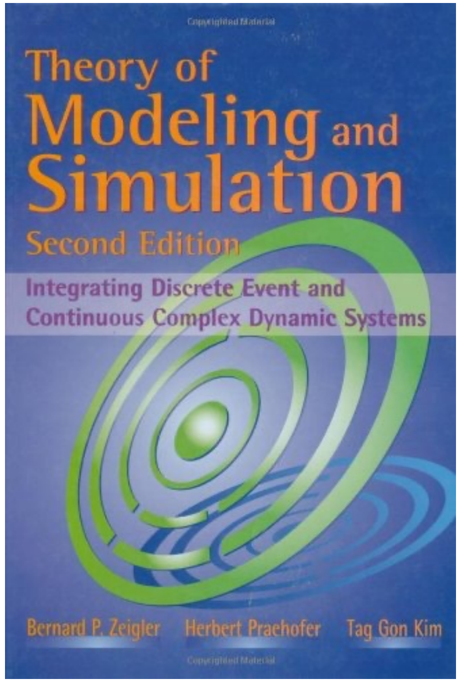
Experimental Frames

The conditions under which the system is observed and experimented with

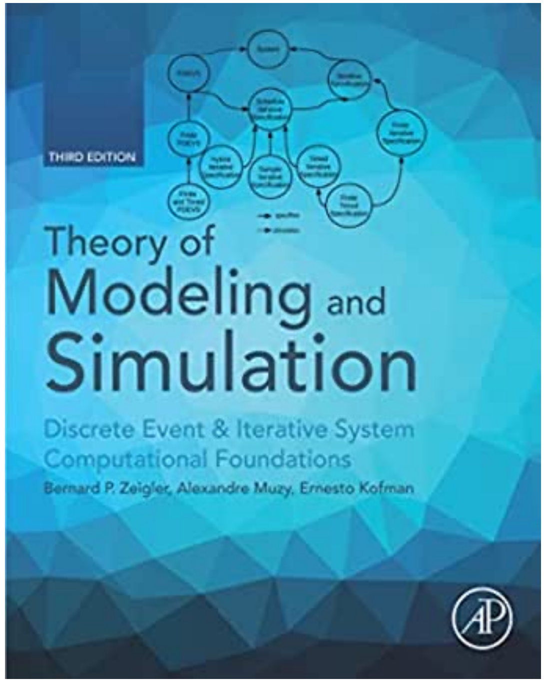
1976



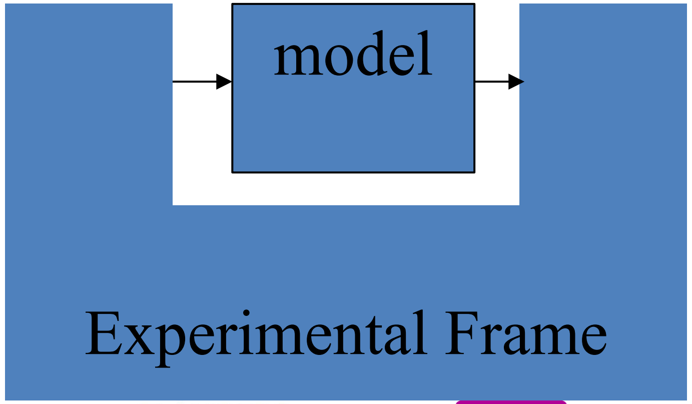
2000



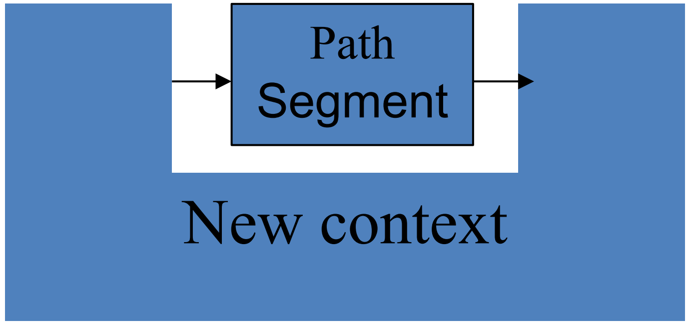
2018

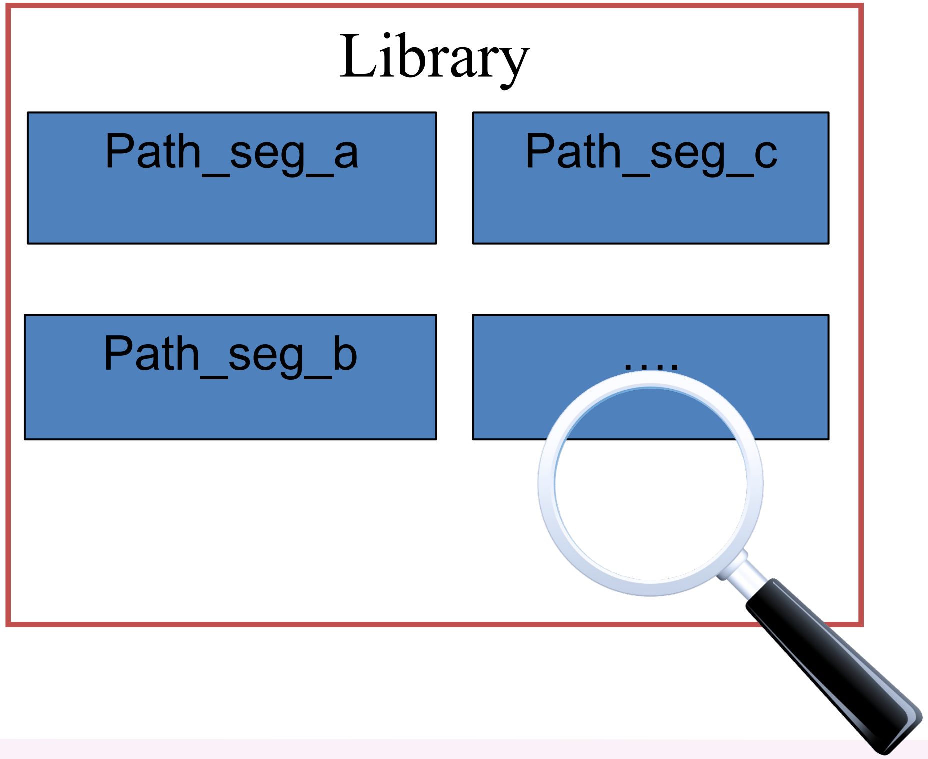


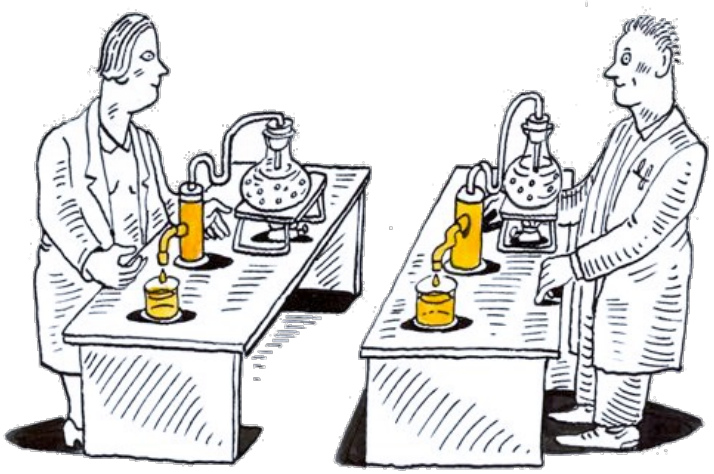
- Making explicit contextual assumptions
- Dual view: meta-data and operationalisation



Uses of the experimental frame







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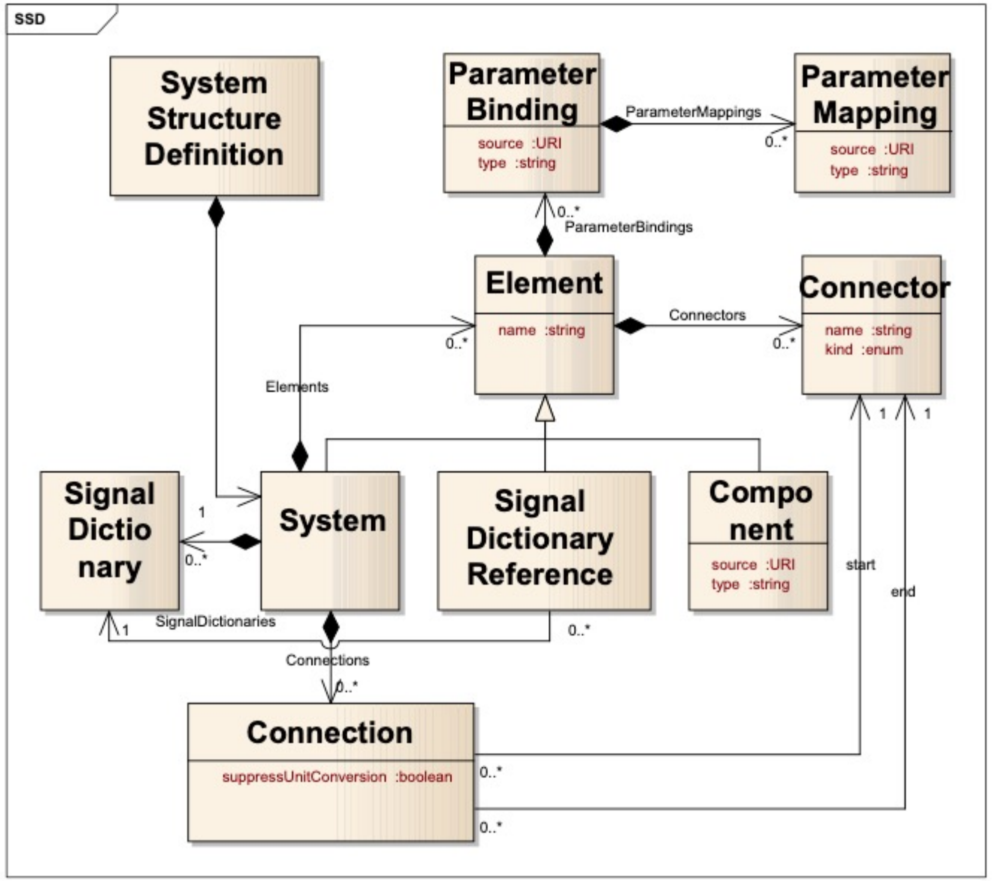
System Structure and Parameterisation (SSP)

standard to define:

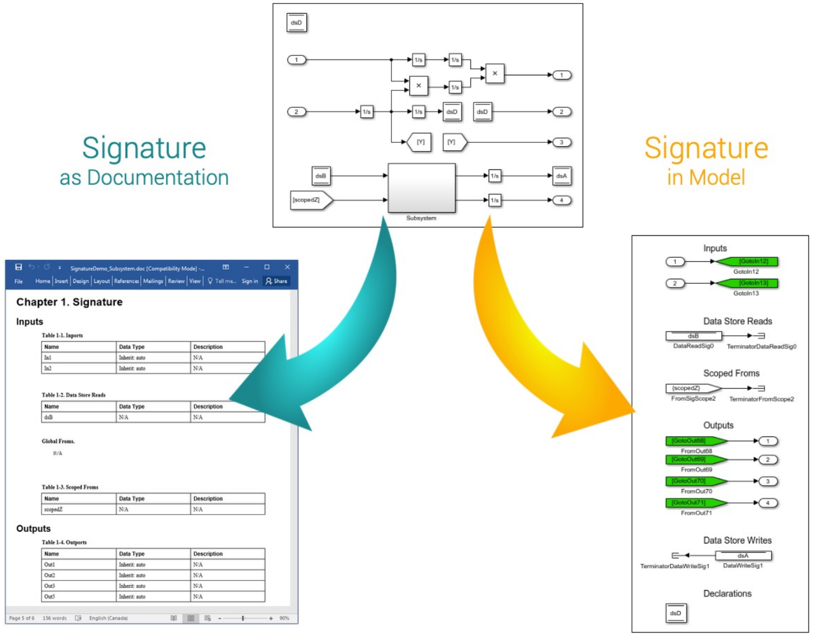
- *complete systems - one or more FMUs*
- *its parameterization*



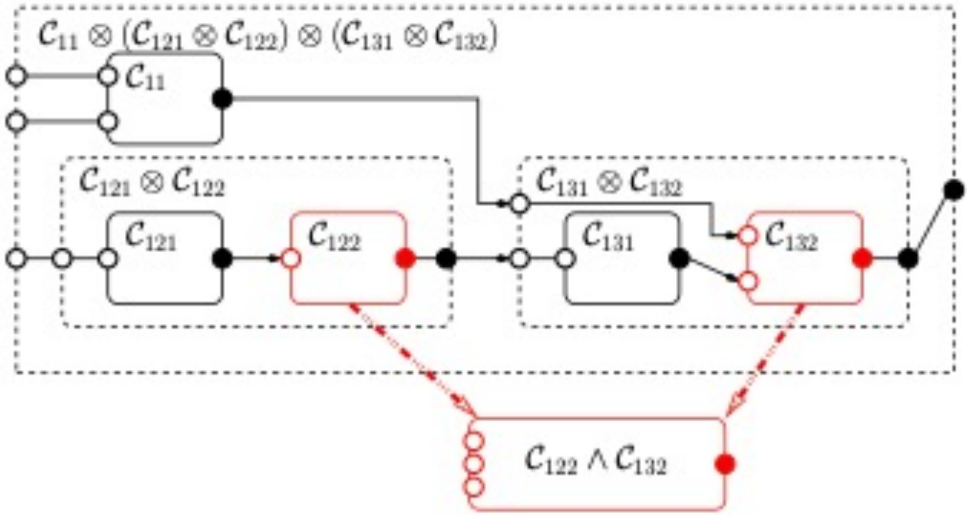
From: Presentation: Deppe et al, MAP " SSP = Current Status and Plans", MA User group meeting, 2018

- Dimensional consistency
- Could allow for structure verification, parameter verification, and boundary condition adequacy

Model Signatures and Contracts



From: Marc Bender, Karen Laurin, Mark Lawford, Vera Pantelic, Alexandre Korobkine, Jeff Ong, Bennett Mackenzie, Monika Bialy, Steven Postma, “Signature required: Making Simulink data flow and interfaces explicit,” Science of Computer Programming, Elsevier, 2015, 113, Part 1, 29-50.



Benveniste, A., Caillaud, B., Nickovic, D., Passerone, R., Raclet, J. B., Reinkemeier, P., ... & Larsen, K. G. (2018). Contracts for system design. *Foundations and Trends® in Electronic Design Automation*, *12*(2-3), 124-400

- Dimensional Consistency
- Internal Structure Verification

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Model Identification Cards

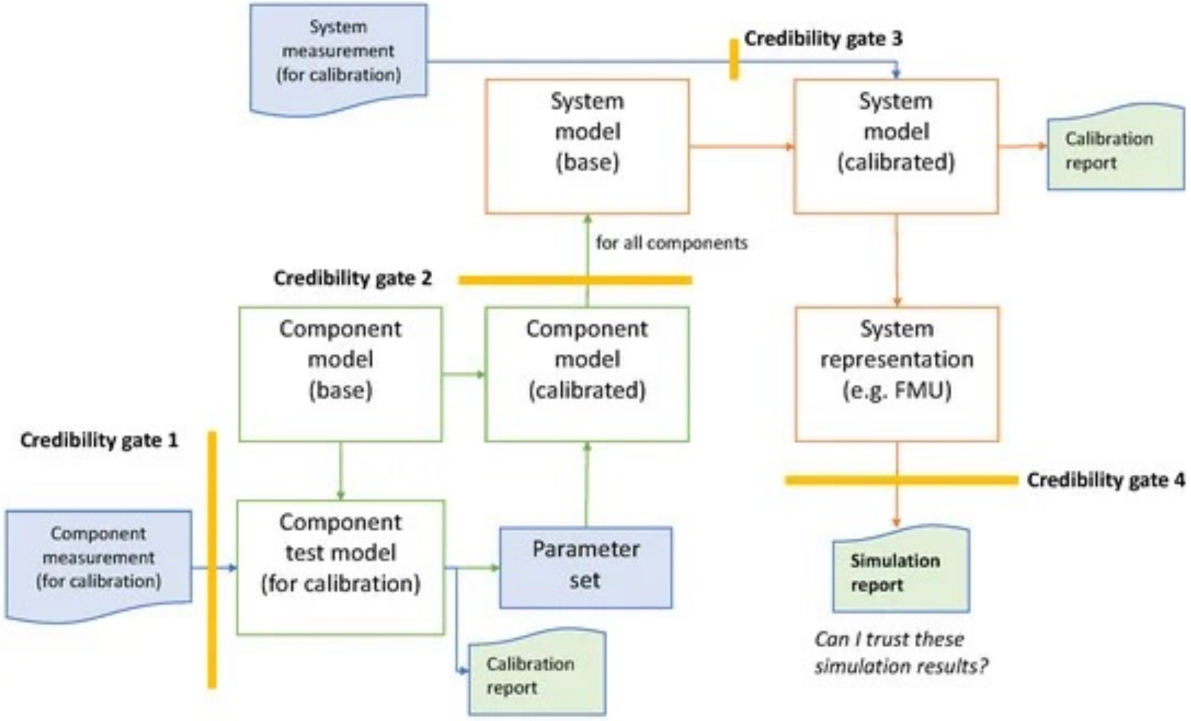
Attributes	Remarques	Type	Example	Main Classes
Generic Name *	Physical componant regroupment	String	Engine	Object Description
Specific Name *	Unique identifier	String	Compressor 7V16	
Granularity Level *	List(System/Sub-system/Componant)	String	Sub-System	
Developer Name *		String	F.Ravet	
Model Version no. *	x.x format	Float	0.1	
Creation Date		Date	14/03/2013	
Documentation	Attached technical report	String		
Image	Attached references image	Image		
Model Dimension	List (0D-3D, mix)	String	1D	Method
Chosen Method	List (Finite Volumes, Finite Elements, Finite Difference, 0D...)	String	Finite Difference	
Physical Equations	List (Chemistry, Dynamic behavior of materials, Maxwell, Navier-Stokes, Strength of materials, Electric, Signal, Runge Kutta)	String	Navier-Stokes	
Integrated Solver	List (Controllable Pitch, Fixed Pitch, Without Solver)	String		
Time Step	List (Second, Minute, Mili-second, Hour, Steady state)	String	Second	
Linearity	List (No/Yes)	String	No	
Discontuntity	List (Yes, No)	String	Yes	

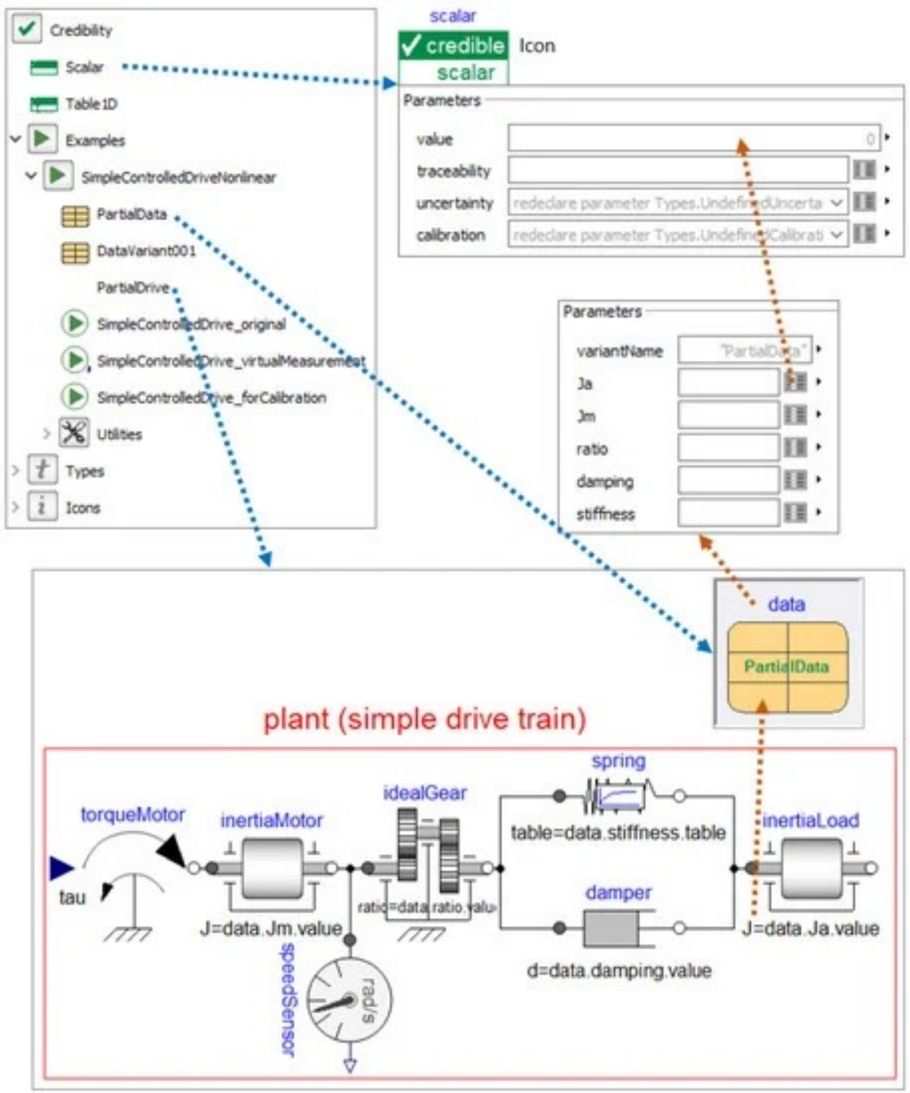
Attributes	Remarques	Type	Example	Main Classes
Name of Compilator	List ()	String	Yes	Usage
Time Computation	List (Elapsed Time / Real Time)	String	Elapsed Time	
Scalability	List (Yes/No)	String	Yes	
Tool Name	List (Amesim, Matlab Simulink, GT-Power, Modelica...)	String	GT-Power	
Tool Version	x.x format	String	7,3	
Hardware Requirements	CPU, OS etc...	String		
Accuracy	Requested/Provided Accuracy	Float	%+-5	Model Quality
Robustness	Requested/Provided Robustness	String	1	
Software (Code) Verification	List (Candidat/Development/Previous/Reference)	String		
Solution (Mathematical) Verification	Level 1(Poor), Level2 (Satisfactory), Level3 (Good), Level4 (Excellent)	String		
Validation	Level 1(Poor), Level2 (Satisfactory), Level3 (Good), Level4 (Excellent)	String		

- Meta-Data on reproducability
- ’Credibility’ information

Göknur Sirin, Christiaan J.J. Paredis, Bernard Yannou, Eric Coatanéa, Eric Landel, “Model Identification Cards to Support Simulation Model Development Process in a Collaborative Multidisciplinary Design Environment , IEEE Systems Journal, 2015

Modelica ‘Credibility Library’





Meta-data with focus on Parameter Calibration (and its uncertainty)

Otter, M.; Reiner, M.; Tobolář, J.; Gall, L.; Schäfer, M. Towards Modelica Models with Credibility Information. *Electronics* **2022**

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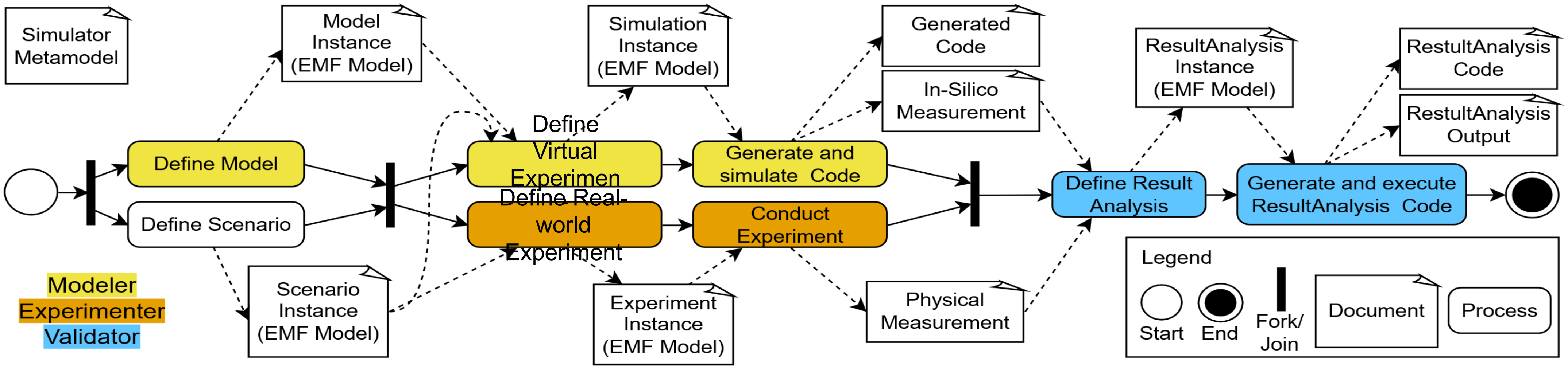
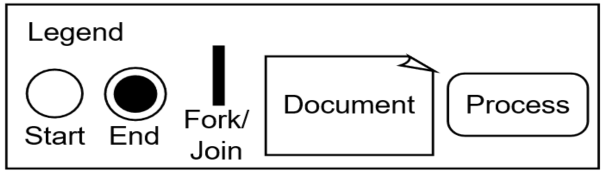
ESS

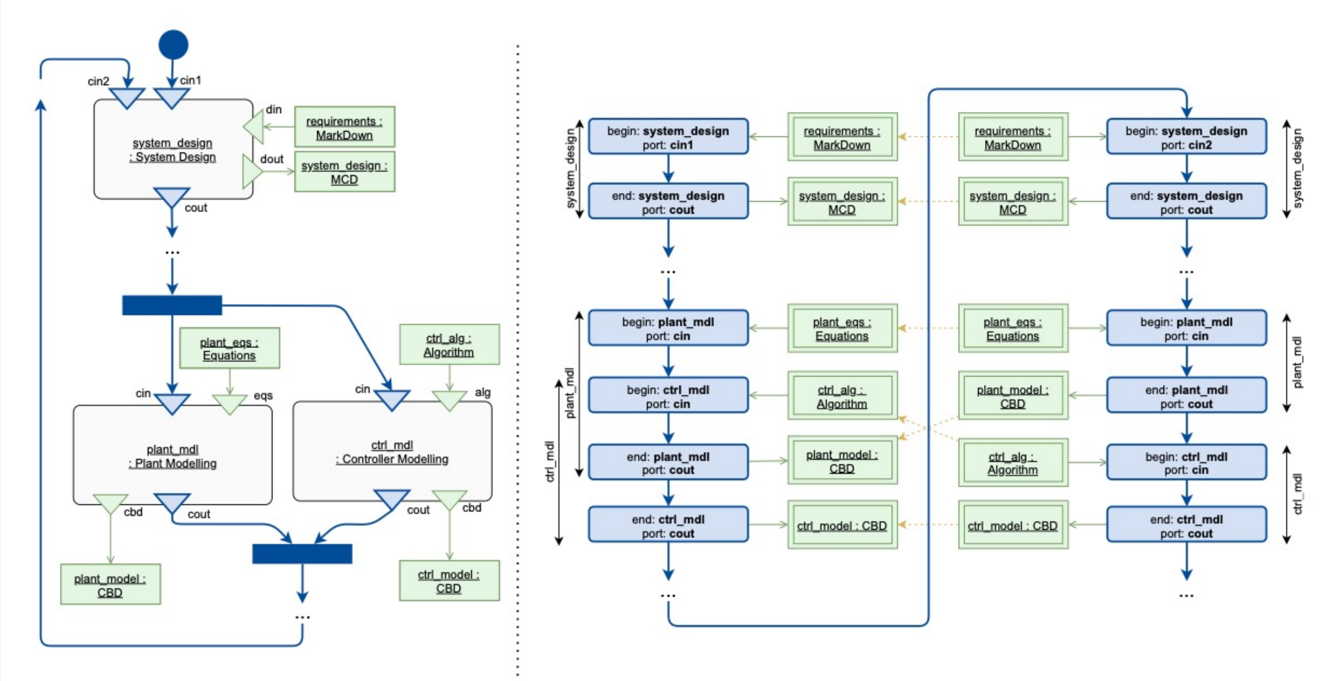




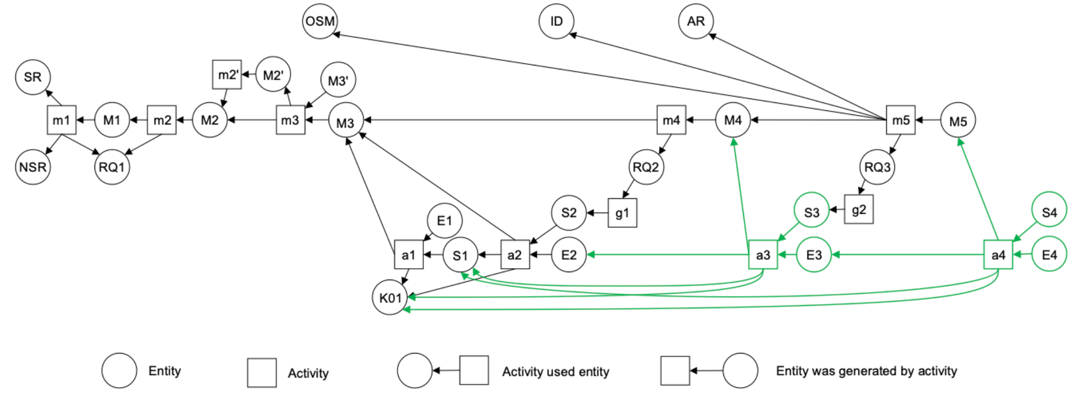
- Experiment Modelling
- Validation Metrics

J. Mertens and J. Denil, "ESS: EMF-Based Simulation Specification, A Domain-Specific Language For Model Validation Experiments," *2022 Annual Modeling and Simulation Conference (ANNSIM)*, 2022

FTG+PM++ and Provenance Models



Paredis, Exelmans, Vangheluwe: MULTI-PARADIGM MODELLING FOR MODEL BASED SYSTEMS ENGINEERING: EXTENDING THE FTG+PM , ANNSIM 2022



P Wilsdorf, A Wolpers, J Hilton, F Haack, AM Uhrmacher, Automatic reuse, adaption, and execution of simulation experiments via provenance patterns, 2022

- Record workflow

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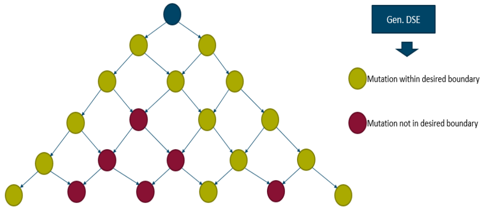
Validity Frames

Meta-information
Enable exploration

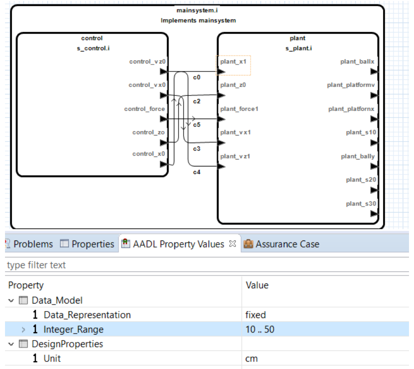
Defines the parameters usable as input for the design space exploration (DSE) or search algorithm



Genetic algorithm for design space exploration

Operational part
Model scope and context

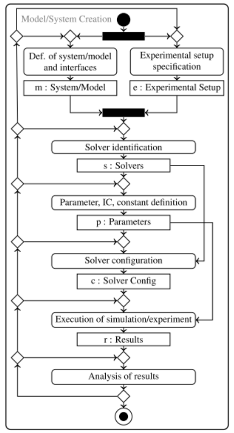
Defines the model scope and context where the model



Run-time monitors!

Process part
Scenario definition

Defines the workflow to perform the allowed scenario's



Source: THE EXPERIMENT MODEL AND VALIDITY FRAME IN M&S

Triple view:

- Meta-data of models (assumptions, solvers, etc.)
- Workflows for calibration, etc.
- Monitors

Van Acker, Bert, et al. "Valid (re-) use of models-of-the-physics in cyber-physical systems using validity frames." *2019 Spring Simulation Conference (SpringSim)*. IEEE, 2019.

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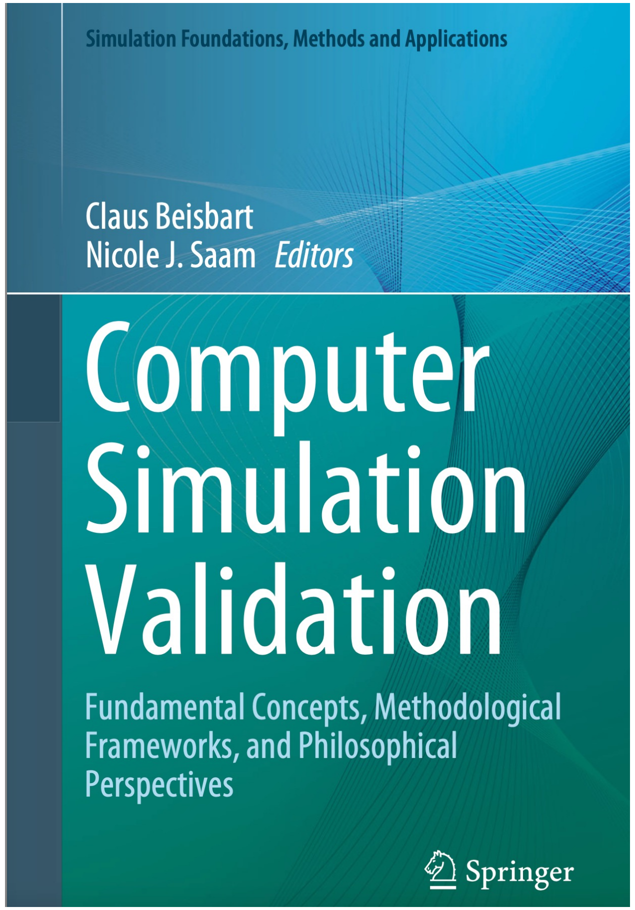
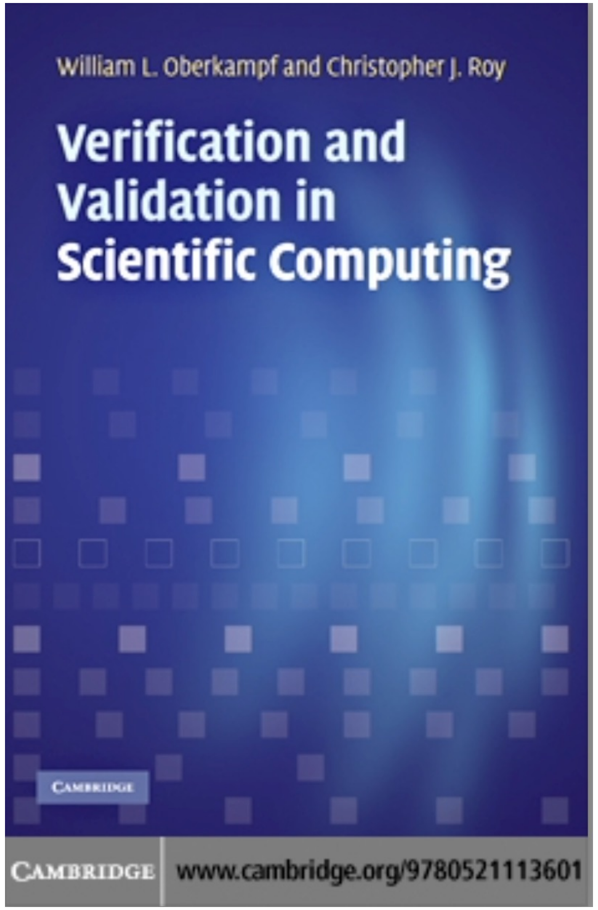
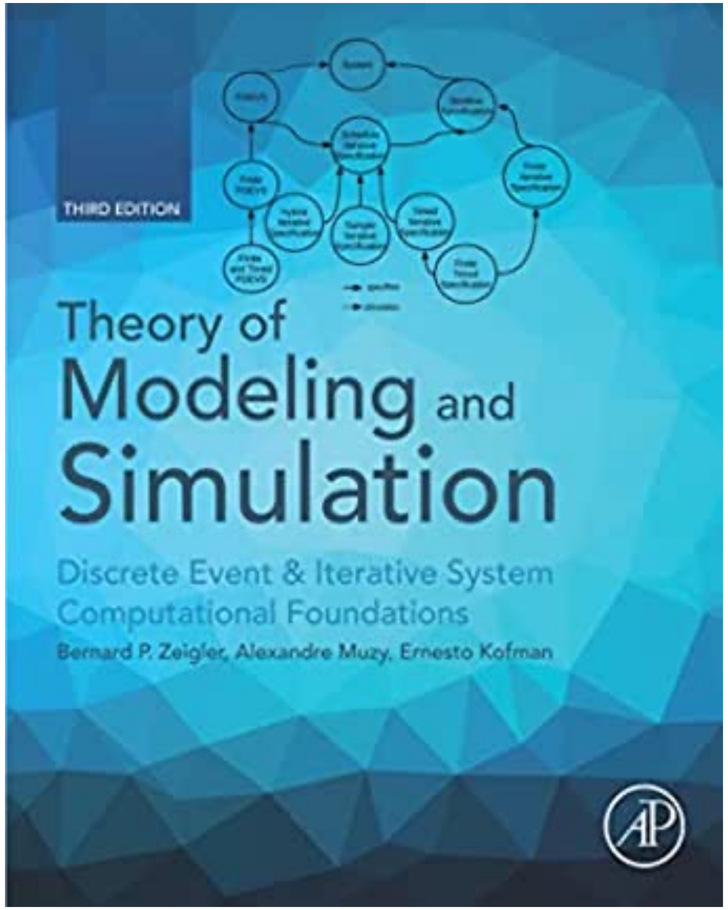
What can we do?

- Standard Monitoring in Models (to check boundary conditions)
  - E.g. FMI could automatically support monitors for run-time validity
- Standard Languages for describing Validity (e.g. MIC, Cred, VF, etc.)
- Tooling for Libraries of Components
  - Searching in Libraries
  - Workflow models embedded for calibration and validity checking

Further Reading







Further Reading (2)

- SMP-2 (ECSS-SMP). ESA standard
- CellML – Simulation Model Metadata