

A Gentle Introduction to Computational Science and Engineering

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Computational Science and Engineering (CSE)

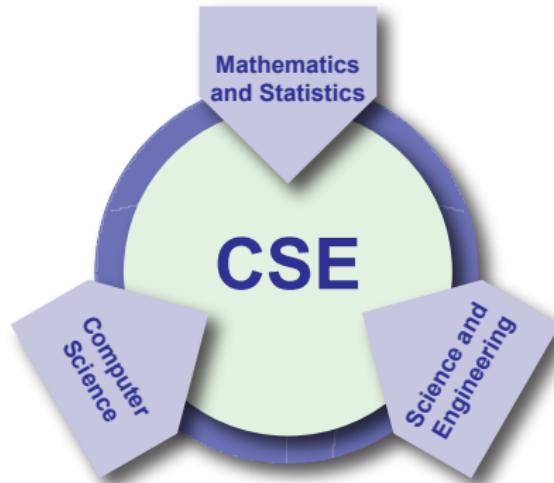
What is CSE?

It is a multidisciplinary area involving:

- applied mathematics
- statistics
- computer science
- science and engineering disciplines

It deals with the development and use of computational methods in sciences, engineering and technology to support:

- discovery
- decision-making



U. Rüde et al., *Research and Education in Computational Science and Engineering*, SIAM Review
Vol. 60, No. 3, pp. 707–754, 2018.

Predictive Science

Four Paradigms for Science

1. Experimental Science

- thousand years ago
- empirical observation/description of natural phenomena

2. Theoretical Science

- last few hundred years
- generalizations via models/mathematical equations

3. Computational Science

- last few decades
- exploration of complex phenomena via computers

4. Data-driven Science

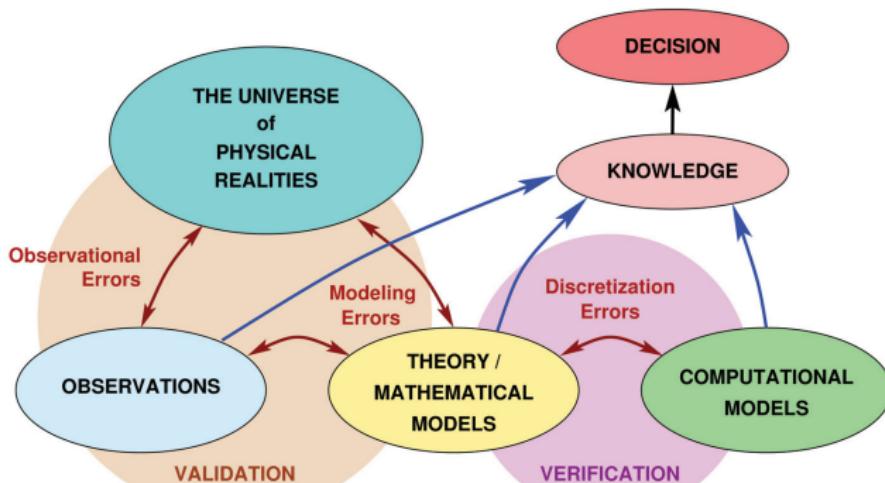
- today
- based on big data sets from several sources
- information extracted via state-of-art statistical methods



T. Hey and S. Tansley and K. Tolle (Editors), *The Fourth Paradigm: Data-Intensive Scientific Discovery*, Microsoft Research, 2009.



The Imperfect Paths to Knowledge

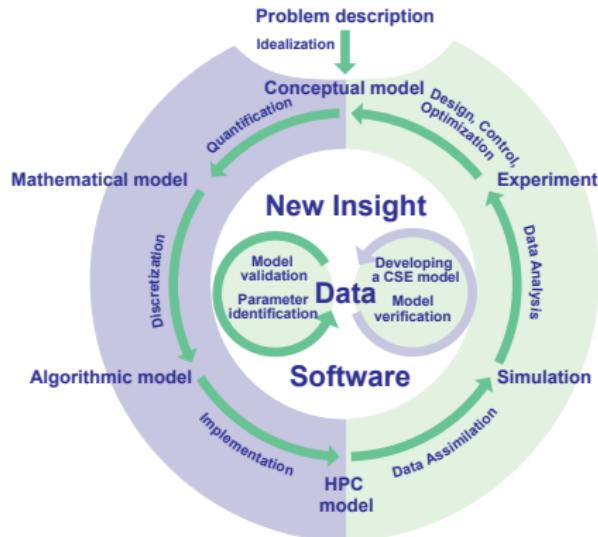


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J. T. Oden et al., *Computer Predictions with Quantified Uncertainty, Part I*. SIAM News, v. 43, 2010.

CSE cycle: from the problem to a new insight



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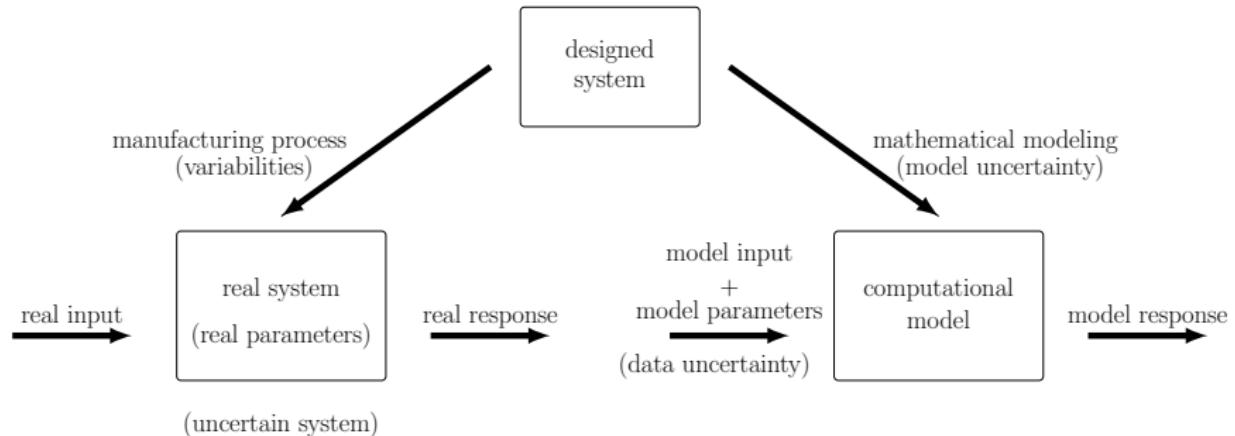
U. Rüde et al., *Research and Education in Computational Science and Engineering*, SIAM Review
Vol. 60, No. 3, pp. 707–754, 2018.



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A Gentle Introduction to Computational Science and Engineering

Computational Prediction: the engineer's perspective



C. Soize, *A comprehensive overview of a non-parametric probabilistic approach of model uncertainties for predictive models in structural dynamics*. *Journal of Sound and Vibration*, 288: 623–652, 2005.



Mathematical Modeling

Model vs Reality

- Reality is too complex to be understood in every detail
- Reality is partially understood through models
- Models are idealizations of reality

Model \neq Reality

- Models must capture main features of reality

Model = Caricature of Reality



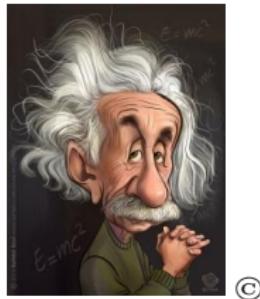
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model

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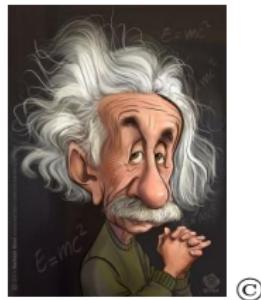
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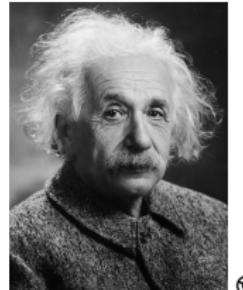
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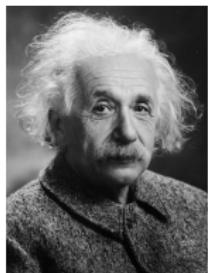
model



reality



For every reality several models are possible



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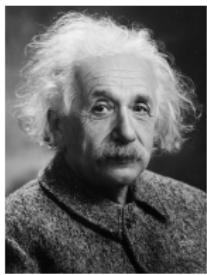
Albert Einstein



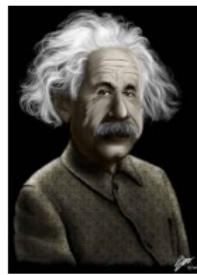
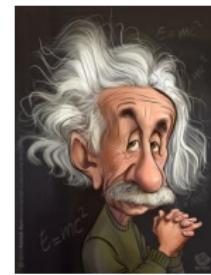
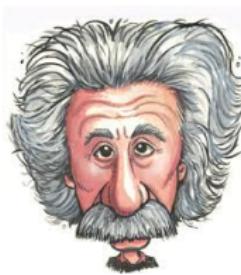
Prof. Samuel da Silva ©

* Samuel authorized his participation!

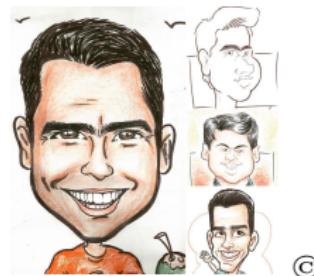
For every reality several models are possible



Albert Einstein



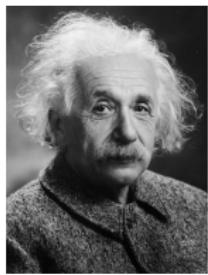
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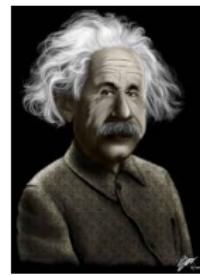
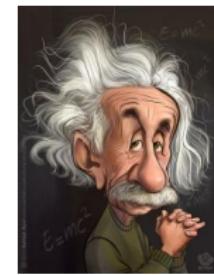
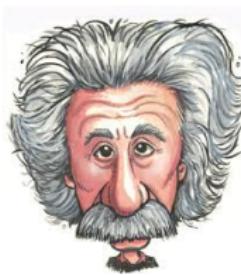
* Samuel authorized his participation!



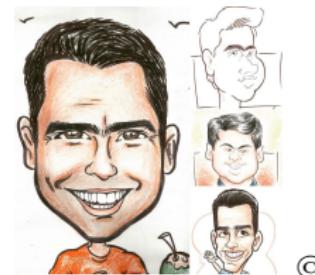
For every reality several models are possible



Albert Einstein



Prof. Samuel da Silva



Models with different levels of fidelity can be constructed!

* Samuel authorized his participation!



Don't think of a model as right or wrong...



*"All models are wrong but
some are useful"*

George E. P. Box

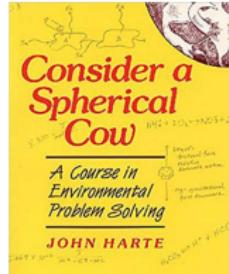


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Forbidden Mango

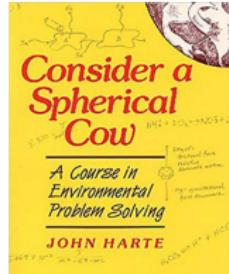


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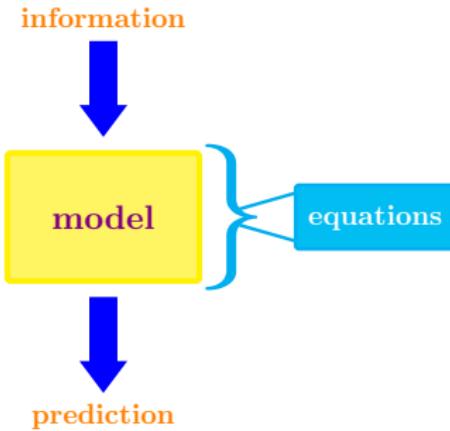
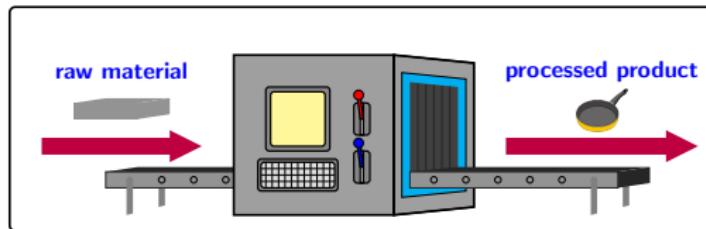
Forbidden Mango



Think a model as useful or not useful!



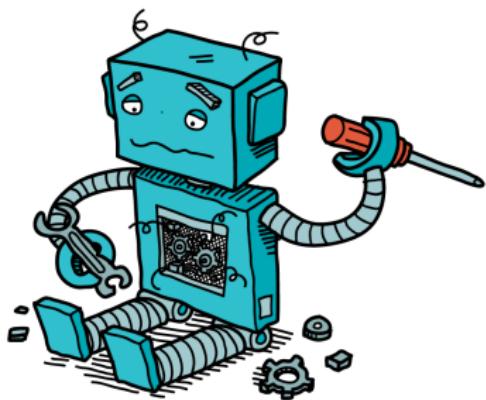
Mathematical model: a predictive “machine”



* Pictures prepared by Michel Tosin.

Mathematical models limitations

- Inappropriate model
(defective machine)
- Poor data
(low quality material)



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*Figures obtained in Google Images. Owners, consider their use as a compliment!

Construction of a physical-mathematical model

It is usually a three-step task:

- 1st step: physical modeling
postulate hypotheses about system
- 2nd step: mathematical modeling
translate hypotheses into equations
- 3rd step: computational modeling
discretization of model equations
implementation into a computer code

Hypotheses may be translate into equations via:

- physical laws
- phenomenological relationships
- ad-hoc considerations
- data-driven information



Model example 1: vehicle dynamics

Real system



(C)



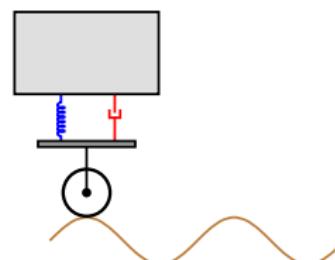
Model example 1: vehicle dynamics

Real system



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Simple model



$$m \ddot{z}(t) + c \dot{z}(t) + k z(t) = F \sin(\omega t)$$

* Simple model picture by Michel Tosin.



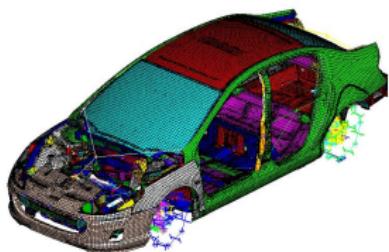
Model example 1: vehicle dynamics

Real system



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Complex model



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$$\rho \vec{\ddot{u}} + c \vec{\dot{u}} = \nabla \cdot \boldsymbol{\sigma}$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$$

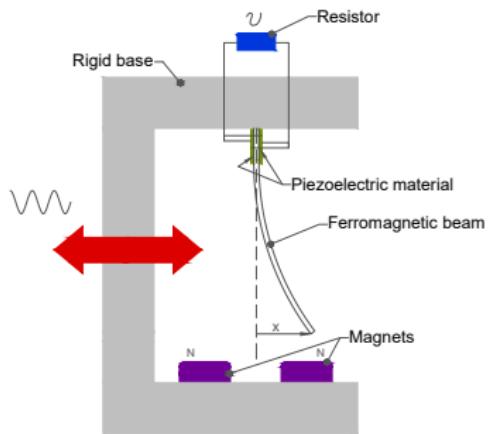
$$2\boldsymbol{\epsilon} = \nabla \mathbf{u} + \nabla \mathbf{u}^T$$

$$\boldsymbol{\sigma} = \mathcal{C} : \boldsymbol{\epsilon}$$

+ b.c./i.c.



Model example 2: piezo-magneto-elastic beam



$$\ddot{x} + 2\xi\dot{x} - \frac{1}{2}x(1-x^2) - \chi v = f \cos \Omega t$$

$$\dot{v} + \lambda v + \kappa \dot{x} = 0$$

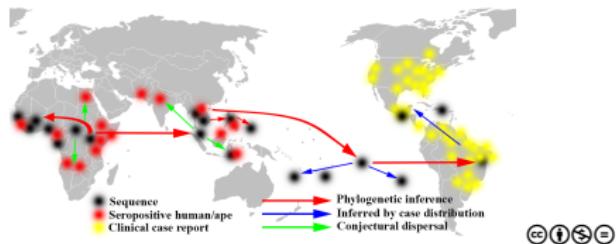
$$x(0) = x_0, \dot{x}(0) = \dot{x}_0, v(0) = v_0$$



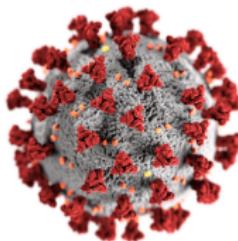
V. Lopes, J. V. L. L. Peterson, and A. Cunha Jr, *Nonlinear characterization of a bistable energy harvester dynamical system*, In: **Topics in Nonlinear Mechanics and Physics: Selected Papers from CSNDD 2018**, Editor: M. Belhaq, Springer Singapore, pp.71-88, 2019.



Model example 3: epidemiological forecast



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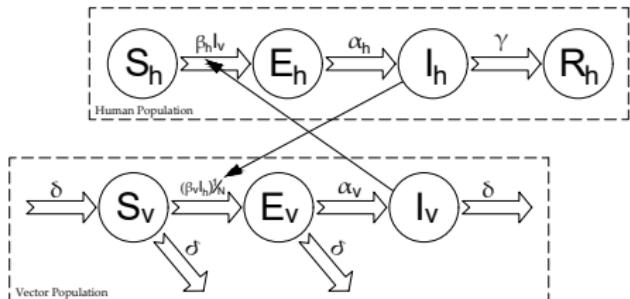


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* Word Cloud generated by <https://www.jasondavies.com/wordcloud>

Model example 3: epidemiological forecast



$$\frac{dS_h}{dt} = -\beta_h S_h I_v$$

$$\frac{dS_v}{dt} = \delta - \beta_v S_v \frac{I_h}{N} - \delta S_v$$

$$\frac{dE_h}{dt} = \beta_h S_h I_v - \alpha_h E_h$$

$$\frac{dE_v}{dt} = \beta_v S_v \frac{I_h}{N} - (\delta + \alpha_v) E_v$$

$$\frac{dI_h}{dt} = \alpha_h E_h - \gamma I_h$$

$$\frac{dI_v}{dt} = \alpha_v E_v - \delta I_v$$

$$\frac{dR_h}{dt} = \gamma I_h$$

$$\frac{dC}{dt} = \alpha_h E_h$$

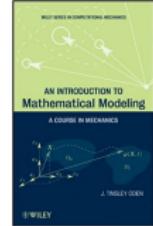
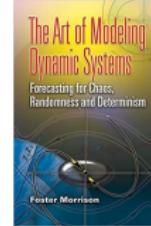
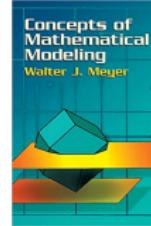
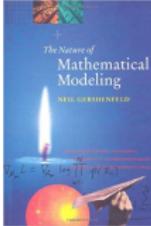
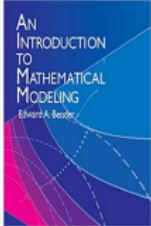
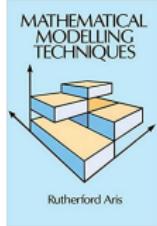
+ initial conditions



E. Dantas, M. Tosin and A. Cunha Jr, *Calibration of a SEIR–SEI epidemic model to describe Zika virus outbreak in Brazil*, *Applied Mathematics and Computations*, vol. 338, pp. 249-259, 2018.

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- Slide 5 – Schematic diagram:
J. T. Oden, *Computer Predictions with Quantified Uncertainty, Part I*. **SIAM News**, v. 43, 2010.
- Slide 6 – CSE cycle diagram:
U. Rüde et al., *Research and Education in Computational Science and Engineering*, **SIAM Review**, v. 60, 2018.
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