A Gentle Introduction to Computational Science and Engineering

Prof. Americo Cunha Jr

Rio de Janeiro State University – UERJ

americo.cunha@uerj.br

www.americocunha.org

@AmericoCunhaJr @AmericoCunhaJr

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Computational Science and Engineering (CSE)

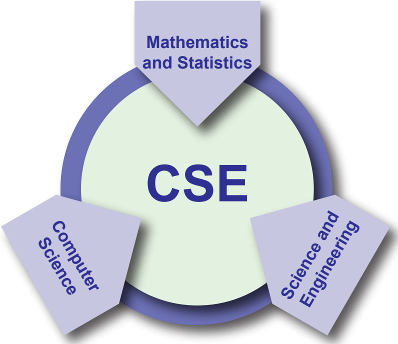
What is CSE?

It is a multidisciplinar 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.

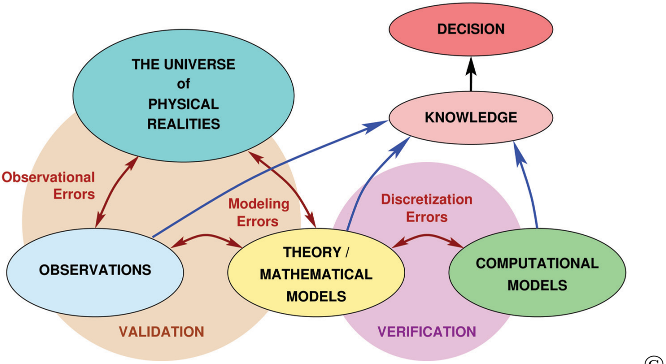
Predictive Science

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

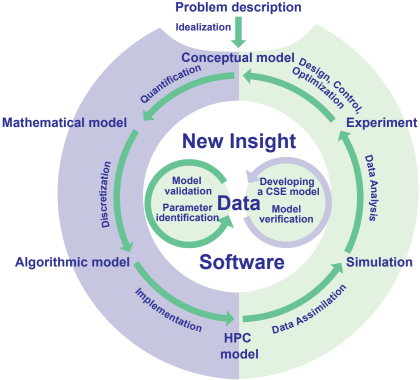
T. Hey and S. Tansley and K. Tolle (Editors), *The Fourth Paradigm: Data-Intensive Scientific Discovery*, Microsoft Research, 2009.

The Imperfect Paths to Knowledge



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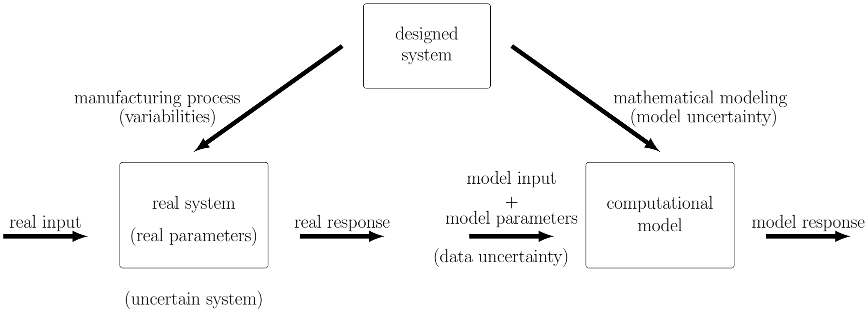
U. Rüde et al., *Research and Education in Computational Science and Engineering*, **SIAM Review** Vol. 60, No. 3, pp. 707–754, 2018.

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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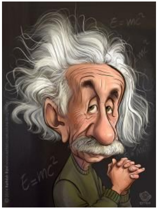

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model

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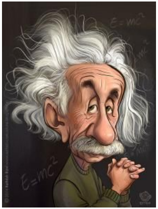

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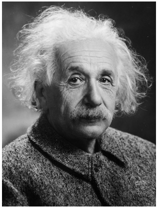
model



reality

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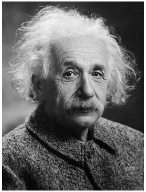
For every reality several models are possible

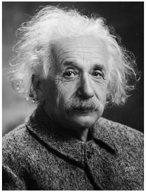


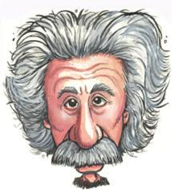
Albert Einstein

Prof. Samuel da Silva ©

* Samuel authorized his participation!

For every reality several models are possible





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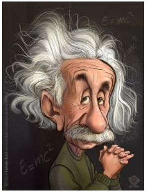

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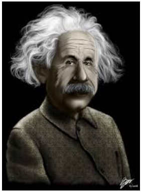

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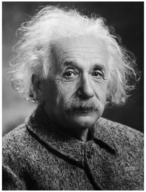

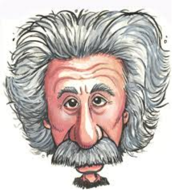
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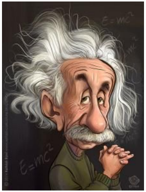
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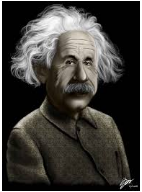
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Albert Einstein

Prof. Samuel da Silva ©


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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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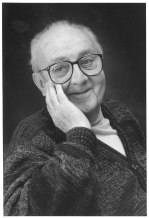
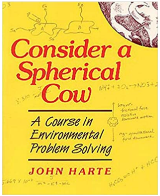


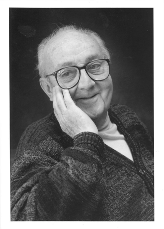
''*All models are wrong but some are useful*''

George E. P. Box



Forbidden Mango

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



"All models are wrong but some are useful"

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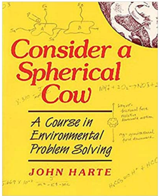

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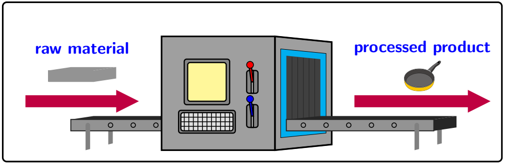
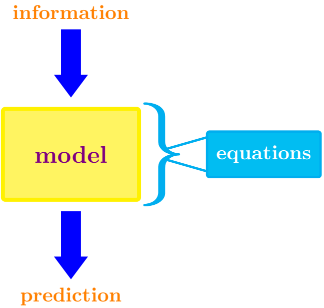
Think a model as useful or not useful!

Mathematical model: a predictive "machine"

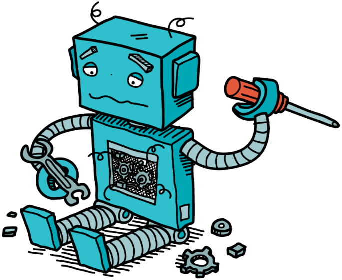




* Pictures prepared by Michel Tosin.

Mathematical models limitations

- Inappropriate model
  (defective machine)



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- Poor data
  (low quality material)

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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

©

Model example 1: vehicle dynamics

Real system

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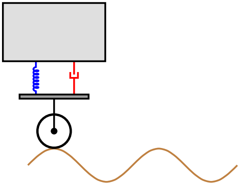
Simple model



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

* Simple model picture by Michel Tosin.

Model example 1: vehicle dynamics

Real system

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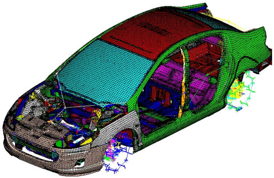
Complex model



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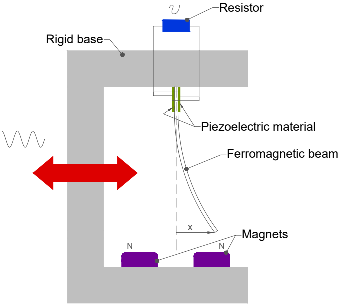
$$
\begin{aligned}
\rho\,\ddot{\vec{u}} + c\,\dot{\vec{u}} &= \nabla \cdot \boldsymbol{\sigma} \\
\boldsymbol{\sigma} &= \boldsymbol{\sigma}^T \\
2\,\epsilon &= \nabla \mathbf{u} + \nabla \mathbf{u}^T \\
\boldsymbol{\sigma} &= \boldsymbol{\mathcal{C}} : \epsilon
\end{aligned}
$$

+ b.c./i.c.

Model example 2: piezo-magneto-elastic beam



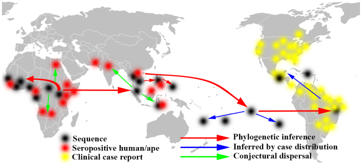
$$\ddot{x} + 2\xi\dot{x} - \frac{1}{2}x(1 - x^2) - \chi\upsilon = f\cos\Omega t$$

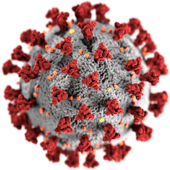
$$\dot{\upsilon} + \lambda\upsilon + \kappa\dot{x} = 0$$

$$x(0) = x_0,\ \dot{x}(0) = \dot{x}_0,\ \upsilon(0) = \upsilon_0$$

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.

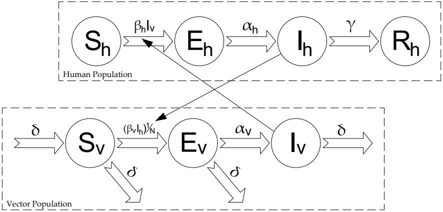
Model example 3: epidemiological forecast





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

Model example 3: epidemiological forecast



$$\frac{d S_h}{dt} = -\beta_h \, S_h \, I_v$$

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

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

$$\frac{d R_h}{dt} = \gamma \, I_h$$

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

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

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

$$\frac{d C}{dt} = \alpha_h \, E_h$$

+ 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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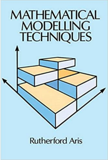
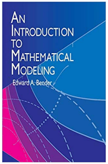
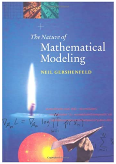
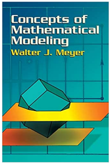
F. Morrison, **The Art of Modeling Dynamic Systems: Forecasting for Chaos, Randomness and Determinism**, Dover Publications; 2nd edition, 2008.

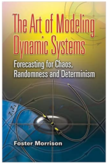
J. Tinsley Oden, **An Introduction to Mathematical Modeling: A Course in Mechanics**, Wiley; 1st edition, 2012.

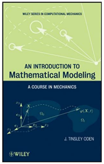












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