A Gentle Introduction to Computational Science and Engineering

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Computational Science and Engineering (CSE)

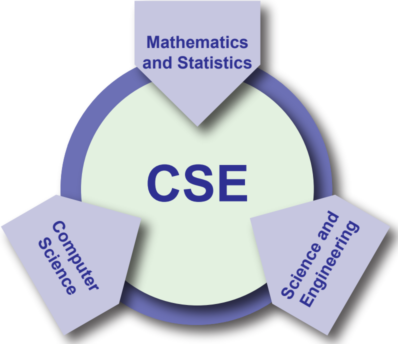
What is CSE?

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.

Computer Science vs Computational Science

Computer Science $\neq$ Computational Science

"Computer science includes all the things we do on our computers and how we build systems to do those kinds of things."

"Computational science is about the application of computers to advance science, largely the modeling and simulating of the physical world."

Prof. Bob Moser, Oden Institute, UT Austin

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

Typical questions on CSE

- What is the best therapy for a patient with a specific disease that minimizes risk and maximizes success probability?
- What are the likely results of hurricanes, tornados, or storm surges on coastal regions, and what plans can be implemented to minimize loss of human life and property?
- How will our climate evolve, and how can we predict outcomes of climate change?

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

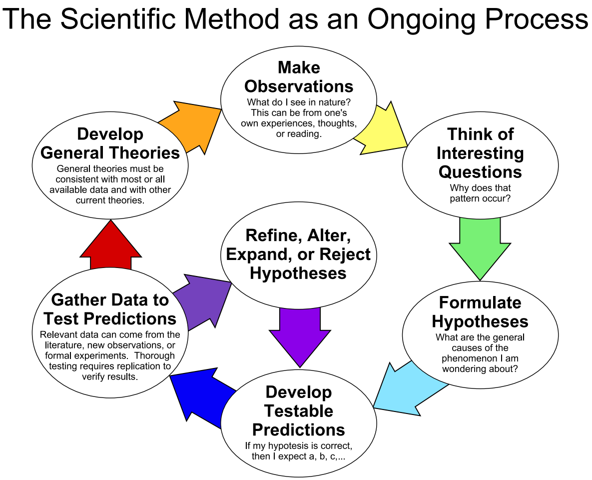
Predictive Science

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

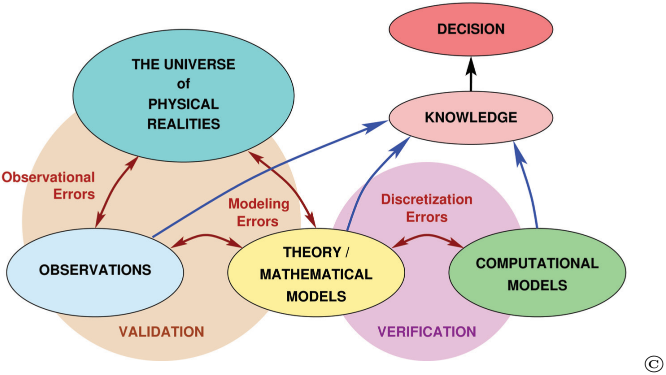
T. Hey and S. Tansley and K. Tolle (Editors), *The Fourth Paradigm: Data-Intensive Scientific Discovery*, Microsoft Research, 2009.

The scientific method



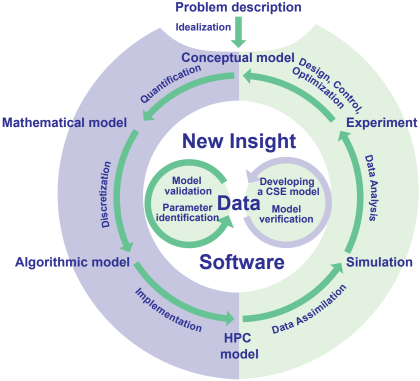
Scientific method, https://en.wikipedia.org/wiki/Scientific_method

The imperfect path to knowledge



J. T. Oden, R. Moser, and O. Ghattas, *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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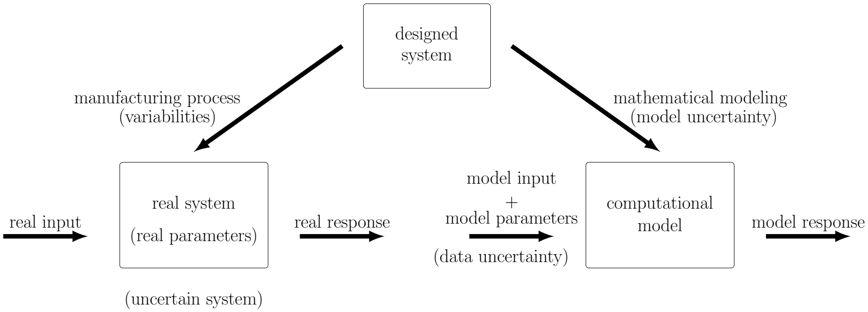
U. Rüde et al., *Research and Education in Computational Science and Engineering*, **SIAM Review** Vol. 60, No. 3, pp. 707–754, 2018.

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.

The Art of Computational Modeling

Model versus Reality

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

$$\textbf{Model} \neq \textbf{Reality}$$

- Models must capture main features of reality

$$\textbf{Model} = \textbf{Caricature of Reality}$$

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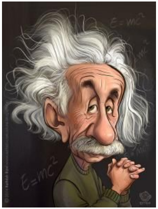

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model

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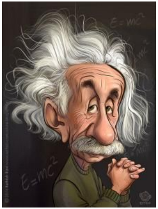

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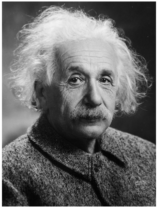
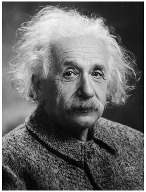
model



reality

For every reality several models are possible

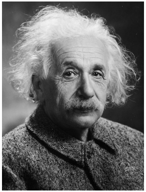


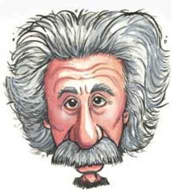
Albert Einstein

Prof. Samuel da Silva ©

* Samuel authorized his participation!

For every reality several models are possible





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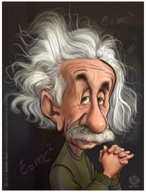

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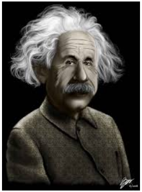

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Albert Einstein

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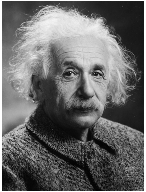
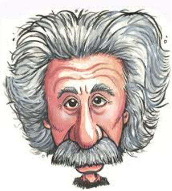
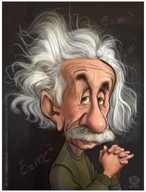
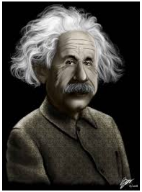
For every reality several models are possible

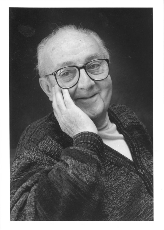
Albert Einstein

Prof. Samuel da Silva ©

Models with different levels of fidelity can be constructed!

* Samuel authorized his participation!

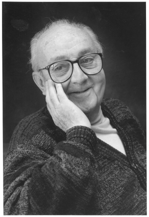
Don't think of a model as right or wrong...



"All models are wrong but some are useful"

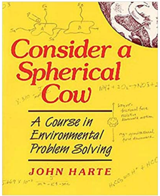
George E. P. Box

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



”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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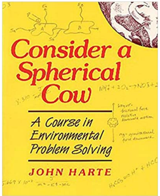
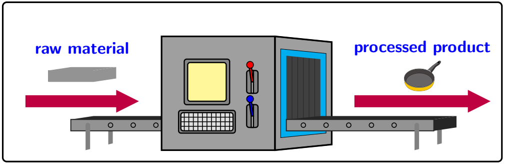
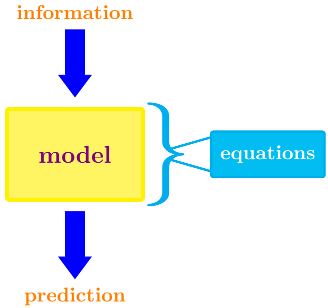


Forbidden Mango

Think a model as useful or not useful!

Computational model: a predictive "machine"

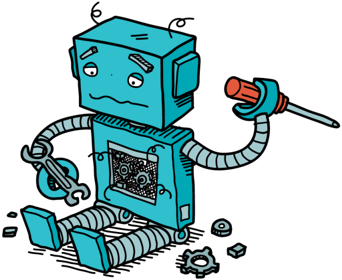




* Pictures prepared by Michel Tosin.

Computational models limitations

- Inappropriate model
  (defective machine)



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- Poor data
  (low quality material)

©

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

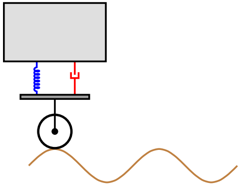
Real system

©

Model example 1: vehicle dynamics

Real system

Simple model



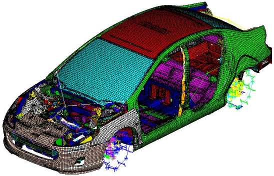
$$m\,\ddot{z}(t) + c\,\dot{z}(t) + k\,z(t) = F\,sin(\omega\,t)$$

* Simple model picture by Michel Tosin.

Model example 1: vehicle dynamics

Real system

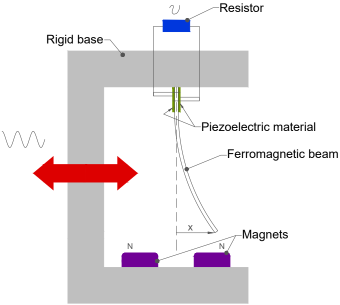
Complex model



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

$+$ b.c./i.c.

Model example 2: piezo-magneto-elastic beam



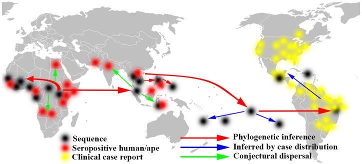
$$\ddot{x} + 2\xi\dot{x} - \frac{1}{2}x(1 - x^2) - \chi v = f\cos\Omega t$$

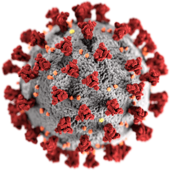
$$\dot{v} + \lambda v + \kappa\dot{x} = 0$$

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

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.

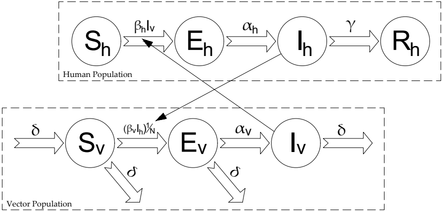
Model example 3: epidemiological forecast





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

Model example 3: epidemiological forecast



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

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

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

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

+ initial conditions

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

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

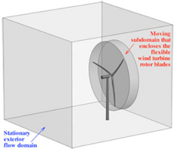
$$\frac{dI_v}{dt} = \alpha_v\, E_v - \delta\, I_v$$

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

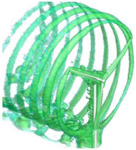
E. Dantas, M. Tosin and A. Cunha Jr, *Calibration of a SEIR–SEI epidemic model to describe Zika virus outbreak in Brazil*, **Applied Mathematics and Computations**, vol. 338, pp. 249-259, 2018.

Some Achievements of CSE

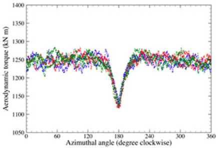
Design of complex engineered systems



(a) Methodology



(b) FSI Simulation



(c) Rotor-Tower Interaction

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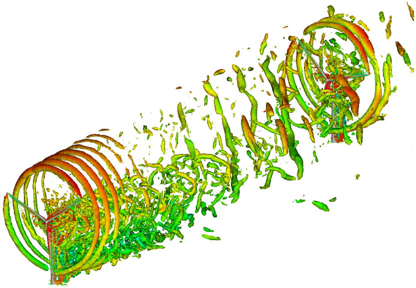

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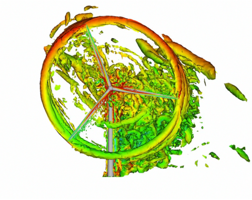

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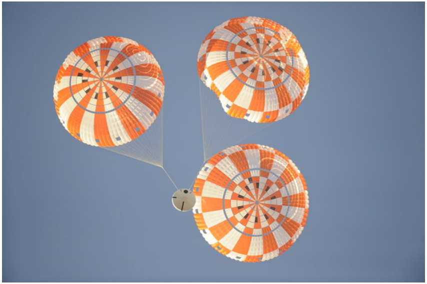
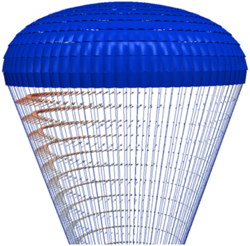
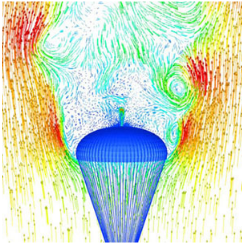
A. Korobenkoa, S. M. I. Goharic, S. Sarkarc and Y. Bazilevs, *FSI Simulation of two back-to-back wind turbines in atmospheric boundary layer flow*. **Computers & Fluids**, v. 158, pp. 167-175, 2017.

Simulation of spacecraft vehicles

NASA Orion Spacecraft Parachute Test

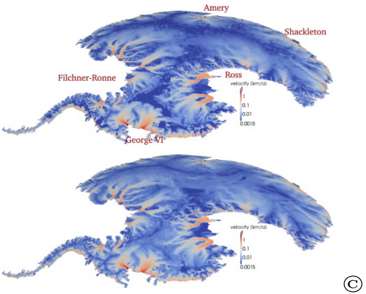


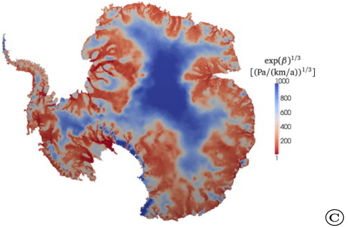


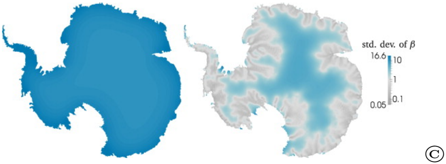


T.E. Tezduyar et al., *Space-Time Finite Element Computation of Complex Fluid-Structure Interactions.* **International Journal for Numerical Methods in Fluids**, 64: 1201-1218, 2010.

Estimation of Antarctic Ice Sheet

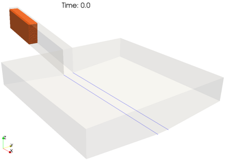


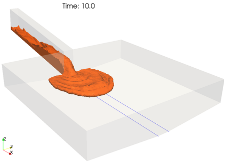


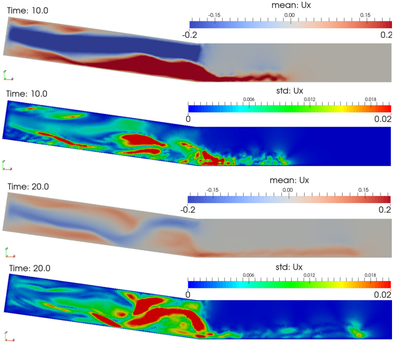


T. Issac, N. Petra, G. Stadler and O. Ghattas, *Scalable and efficient algorithms for the propagation of uncertainty from data through inference to prediction for large-scale problems, with application to flow of the Antarctic ice sheet.* **Journal of Computational Physics**, 296: 348–368, 2015.

Analysis of geological events







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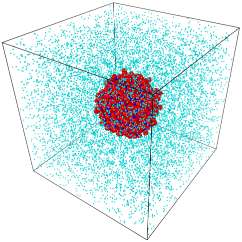
G. M. Guerra, S. Zio, J. J. Camata, J. Dias, R. N. Elias, M. Mattoso, P. L. B. Paraizo, A. L. G. A. Coutinho, F, A. Rochinha, *Uncertainty quantification in numerical simulation of particle-laden flows.* **Computational Geosciences**, 20: 265-281, 2016.

Prediction of nanoscale systems behavior



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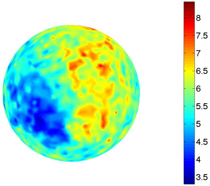

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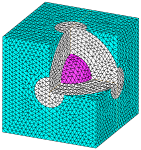

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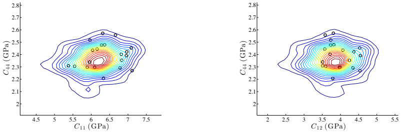

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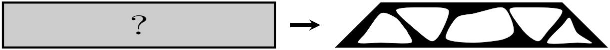
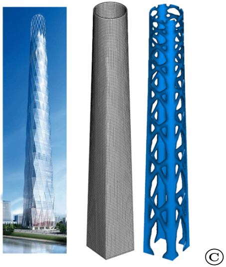
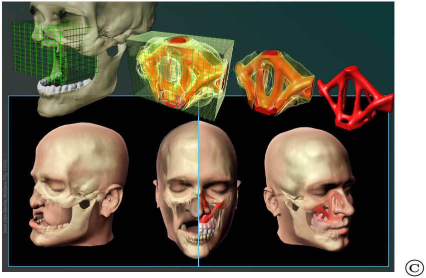
T. Le, J. Guilleminot, and C. Soize. *Stochastic continuum modeling of random interphases from atomistic simulations. Application to a polymer nanocomposite.* **Computer Methods in Applied Mechanics and Engineering**, 303: 430-449, 2016.

Topology optimization in engineering systems



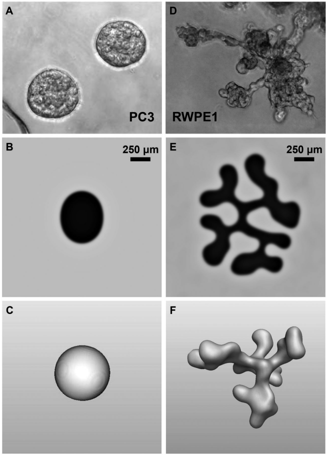




* Pictures adapted from Prof. Gláucio H. Paulino (Georgia Tech) class notes.

Beam-Truss picture prepared by Marcos Vinícius Issa.

Modeling the evolution process of diseases



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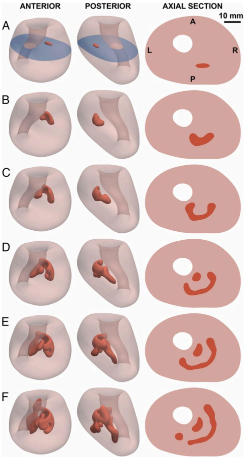

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Remarks on CSE

Some perspectives and challenges on CSE

Perspectives:

- Development of increasingly realistic models
- Frequent use outside engineering

Challenges:

- Data-driven methods to construct high-fidelity models
- Strict procedures for verification of computational codes
- Suitable frameworks for validation of models
- Hardware, software and algorithms for extreme-scale computing

Key points about CSE

- CSE is multidisplinar:
  applied mathematics
  statistics
  computer science
  science and engineering
- CSE is a relatively new discipline
  remarkable achievements have been done
  much more achievements are expected
- Applications of CSE transcend engineering world
  astrophysics
  geosciences
  social sciences
  medical sciences
  ...
- Huge research challenges come with CSE development

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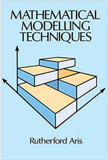

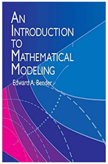

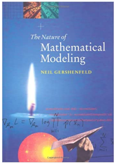

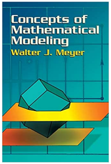

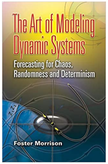

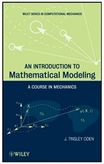

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