

A Gentle Introduction to Computational Science and Engineering

Prof. Americo Cunha Jr

americocunha.org



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Computational Science and Engineering (CSE)

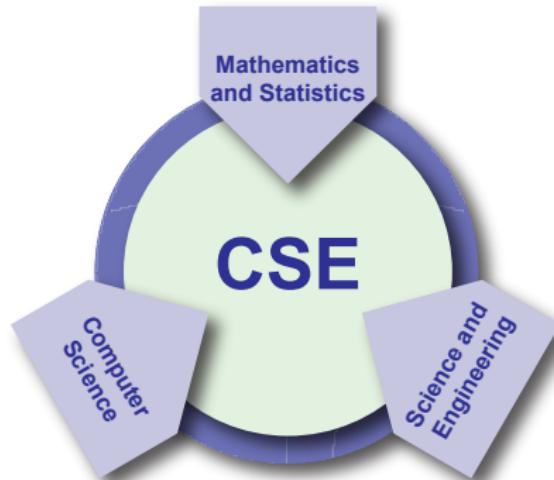
What is CSE?

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.

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

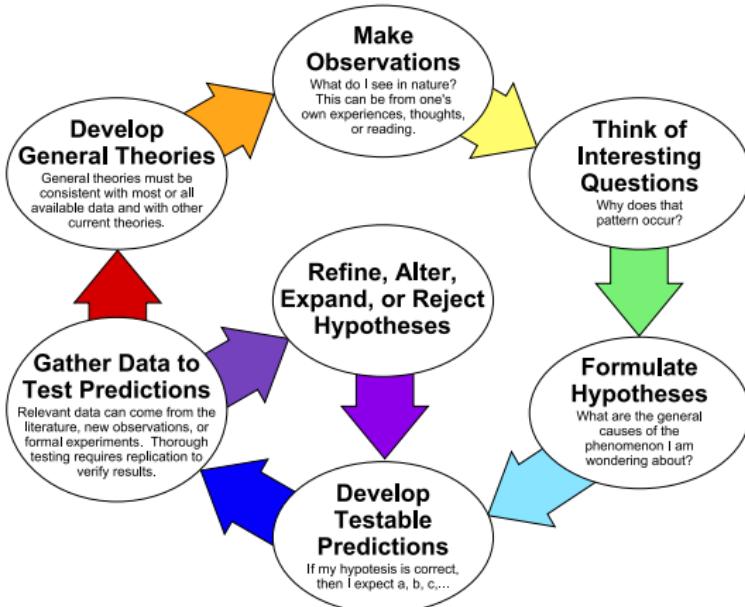
- today
- based on big data sets from several sources
- information extracted via state-of-art statistical methods



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

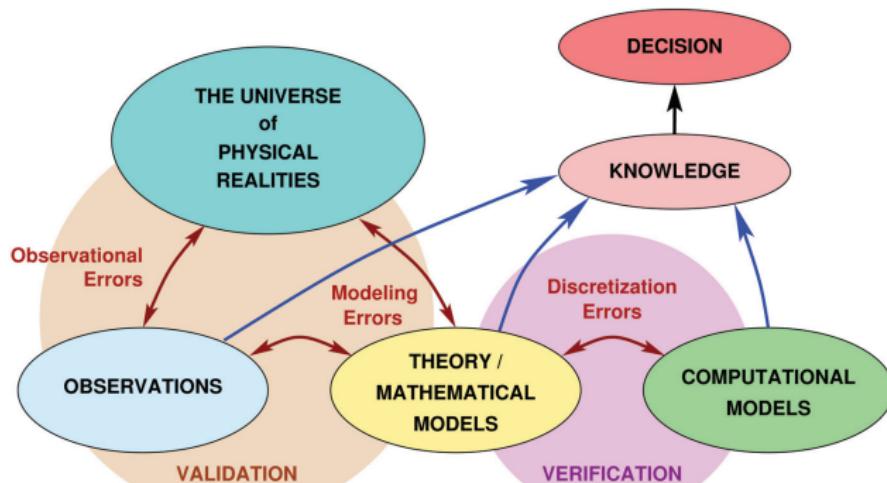
The scientific method

The Scientific Method as an Ongoing Process



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

The imperfect path to knowledge



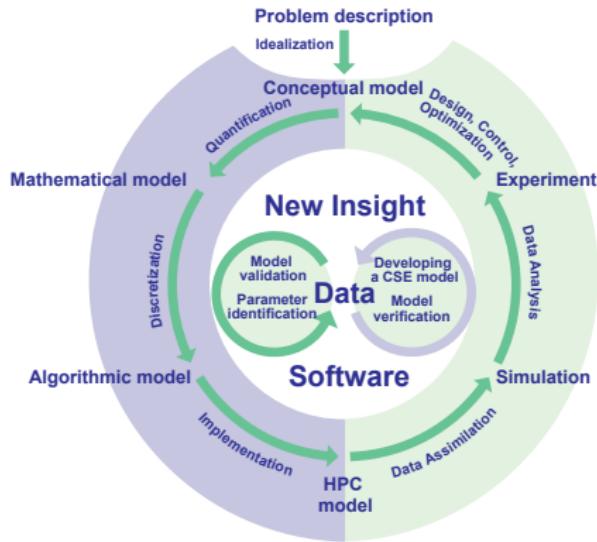
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J. T. Oden, R. Moser, and O. Ghattas, *Computer Predictions with Quantified Uncertainty, Part I.*

SIAM News, v. 43, 2010.

CSE cycle: from the problem to a new insight



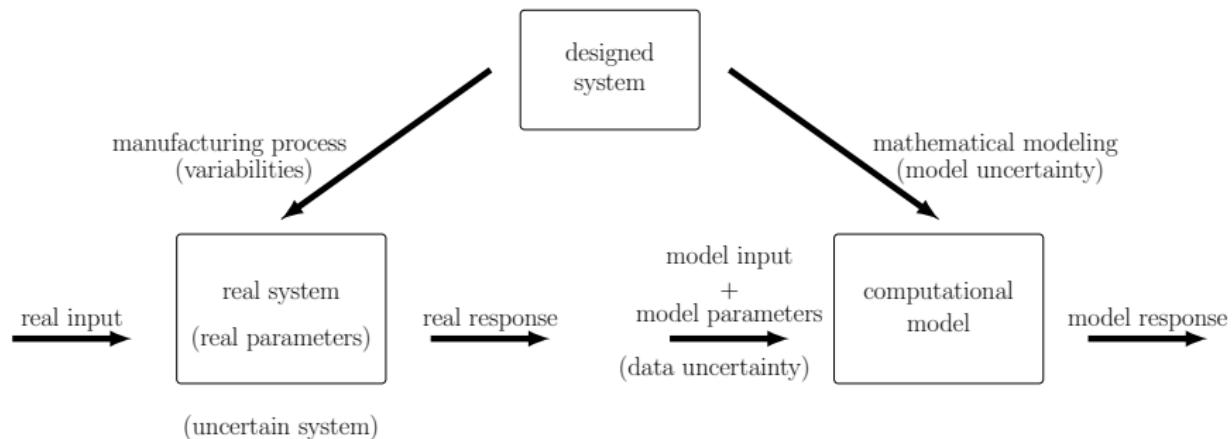
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U. Rüde et al., *Research and Education in Computational Science and Engineering*, SIAM Review

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

Model \neq Reality

- Models must capture main features of reality

Model = Caricature of Reality

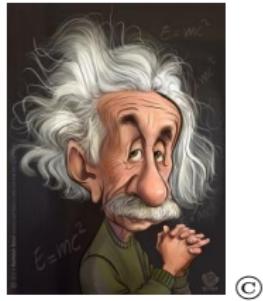
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model

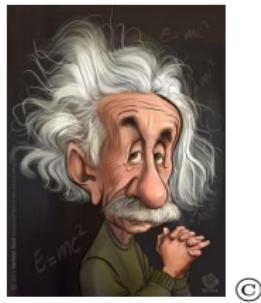
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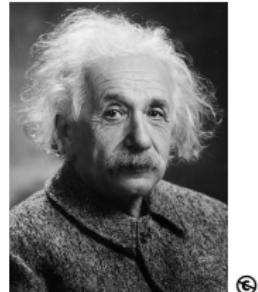
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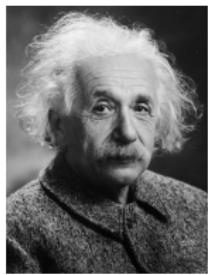


model



reality

For every reality several models are possible



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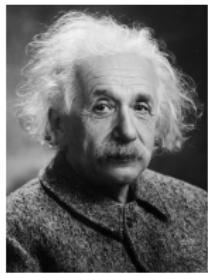
Albert Einstein



Prof. Samuel da Silva ©

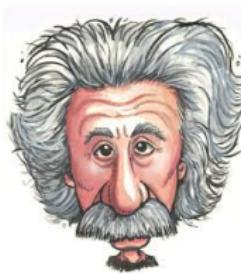
* Samuel authorized his participation!

For every reality several models are possible

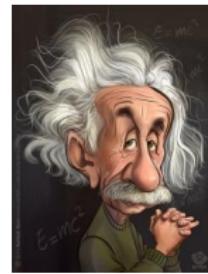


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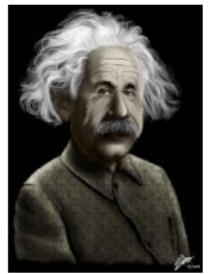
Albert Einstein



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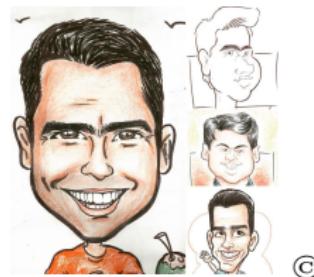
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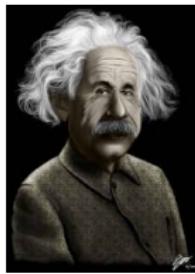
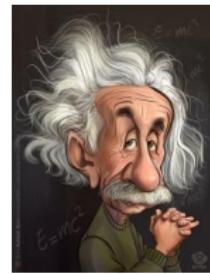
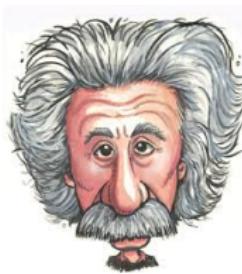
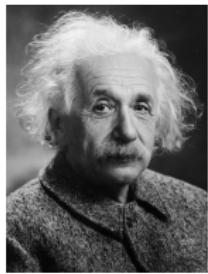


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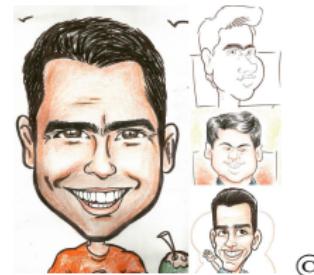
For every reality several models are possible



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...



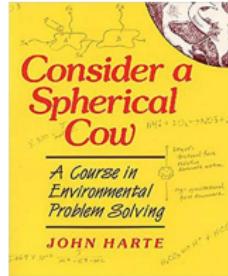
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*"All models are wrong but
some are useful"*

George E. P. Box



CC



CC



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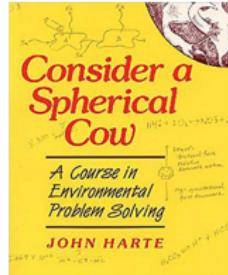
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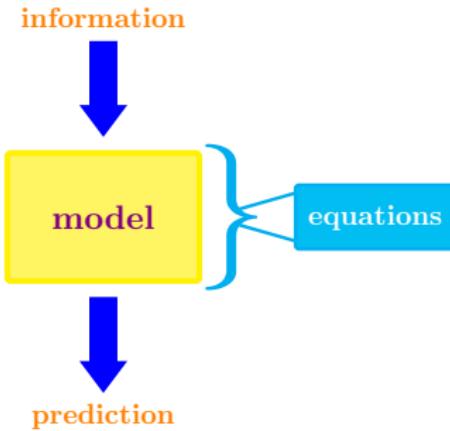
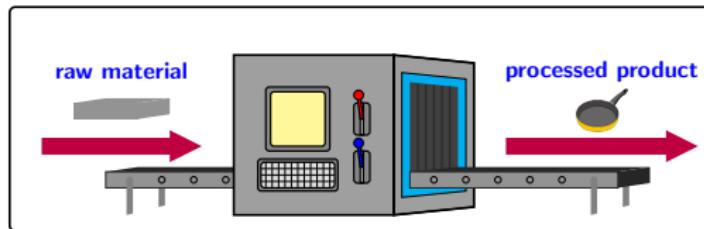


Forbidden Mango



Think a model as useful or not useful!

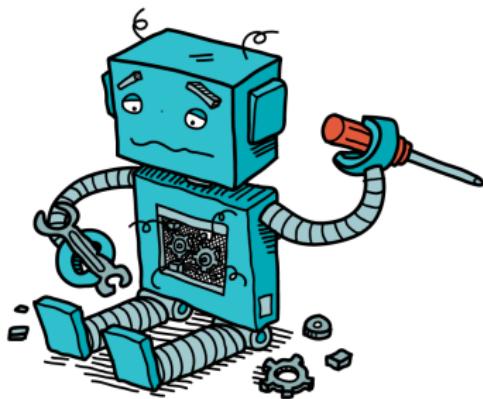
Computational model: a predictive “machine”



* Pictures prepared by Michel Tosin.

Computational models limitations

- Inappropriate model
(defective machine)
- 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



(C)

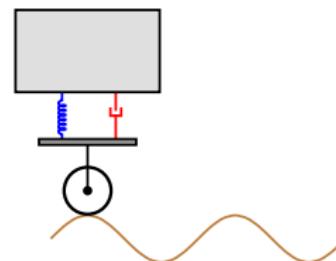
Model example 1: vehicle dynamics

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.

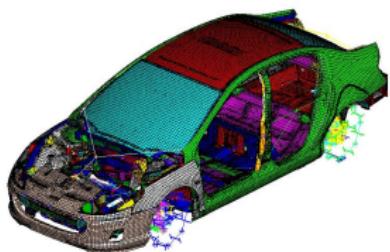
Model example 1: vehicle dynamics

Real system



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Complex model



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

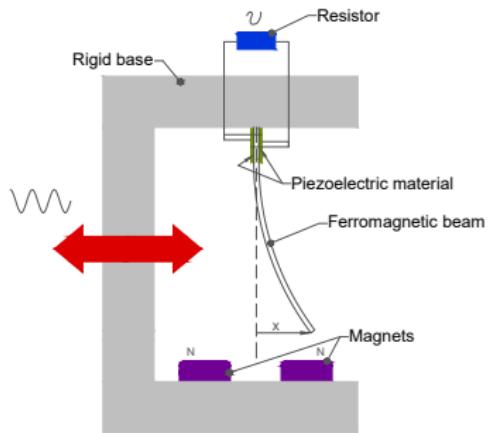
$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$$

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

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

+ b.c./i.c.

Model example 2: piezo-magneto-elastic beam



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

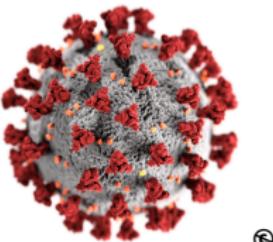
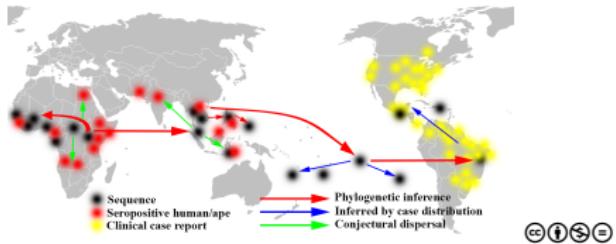
$$\dot{v} + \lambda v + \kappa \dot{x} = 0$$

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



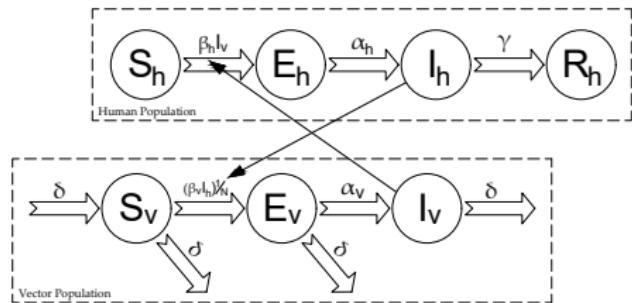
V. Lopes, J. V. L. L. Peterson, and A. Cunha Jr, *Nonlinear characterization of a bistable energy harvester dynamical system*, In: **Topics in Nonlinear Mechanics and Physics: Selected Papers from CSNDD 2018**, Editor: M. Belhaq, Springer Singapore, pp.71-88, 2019.

Model example 3: epidemiological forecast



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

Model example 3: epidemiological forecast



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

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

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

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

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

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

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

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

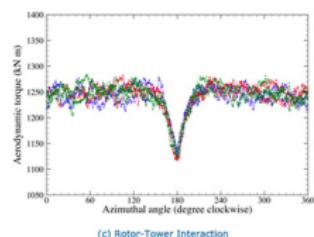
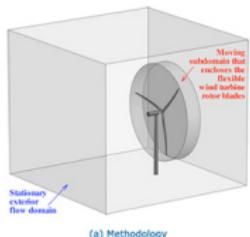
+ initial conditions



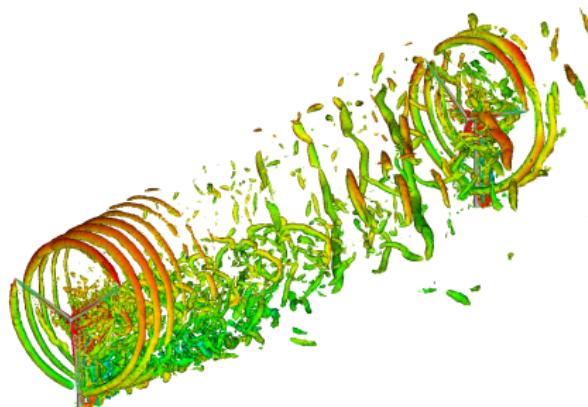
E. Dantas, M. Tosin and A. Cunha Jr, *Calibration of a SEIR–SEI epidemic model to describe Zika virus outbreak in Brazil*, **Applied Mathematics and Computations**, vol. 338, pp. 249-259, 2018.

Some Achievements of CSE

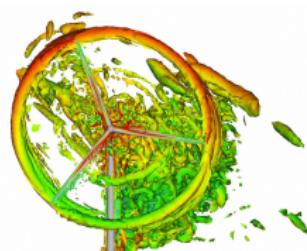
Design of complex engineered systems



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A. Korobenka, 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



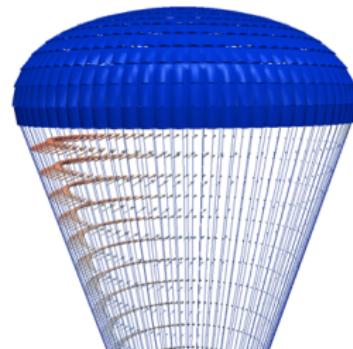
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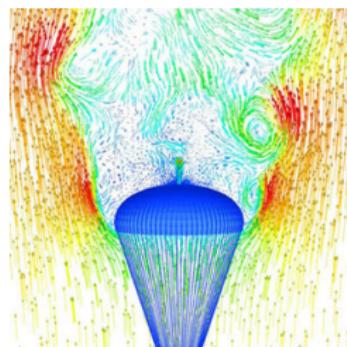
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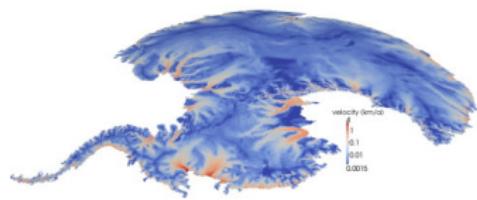
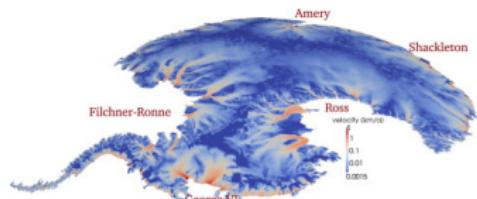


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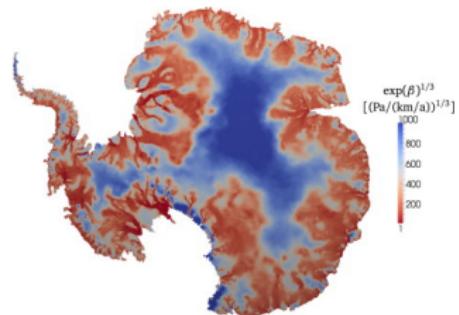


T.E. Tezduyar et al., *Space-Time Finite Element Computation of Complex Fluid-Structure Interactions*. International Journal for Numerical Methods in Fluids, 64: 1201-1218, 2010.

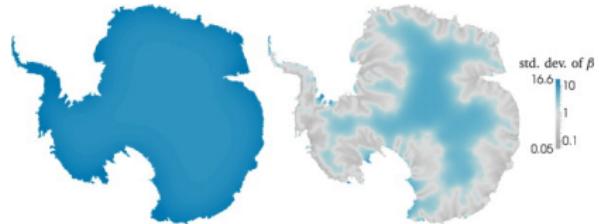
Estimation of Antarctic Ice Sheet



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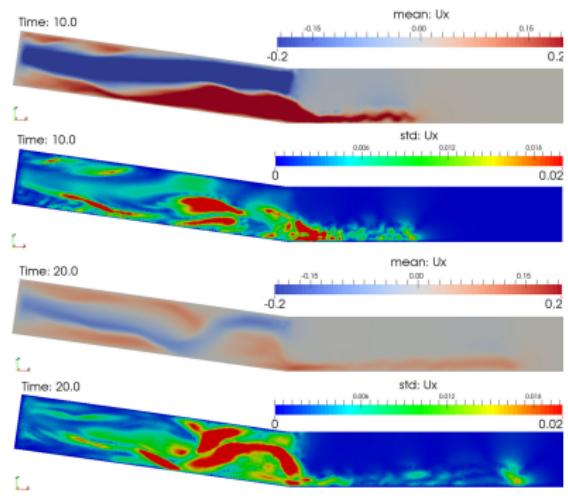
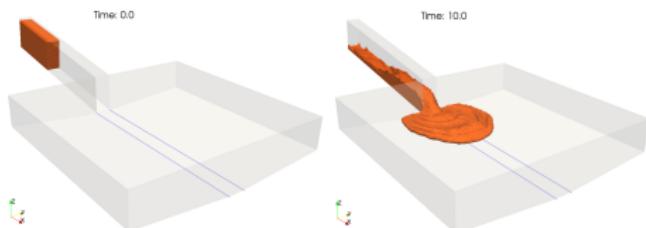


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T. Issac, N. Petra, G. Stadler and O. Ghattas, *Scalable and efficient algorithms for the propagation of uncertainty from data through inference to prediction for large-scale problems, with application to flow of the Antarctic ice sheet*. *Journal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

Analysis of geological events



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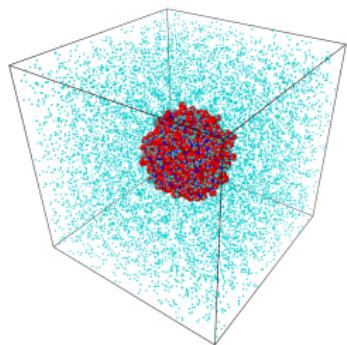


G. M. Guerra, S. Zio, J. J. Camata, J. Dias, R. N. Elias, M. Mattoso, P. L. B. Paraizo, A. L. G. A.

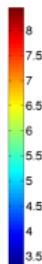
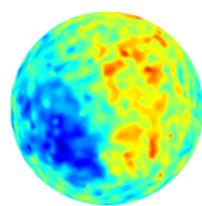
Coutinho, F, A. Rochinha, *Uncertainty quantification in numerical simulation of particle-laden flows.*

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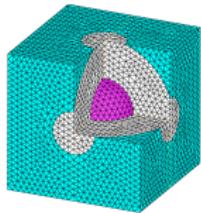
Prediction of nanoscale systems behavior



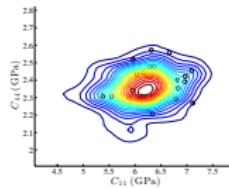
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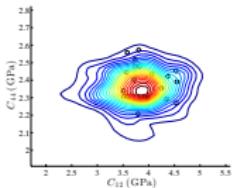
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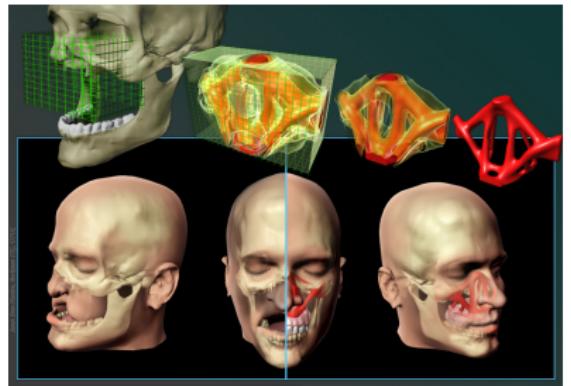


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T. Le, J. Guilleminot, and C. Soize. *Stochastic continuum modeling of random interphases from atomistic simulations. Application to a polymer nanocomposite.* Computer Methods in Applied Mechanics and Engineering, 303: 430-449, 2016.

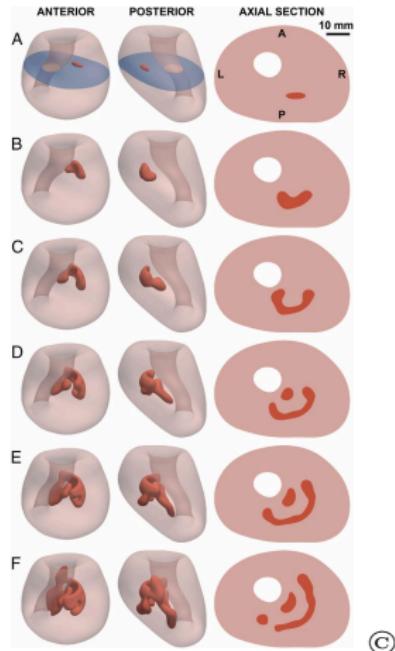
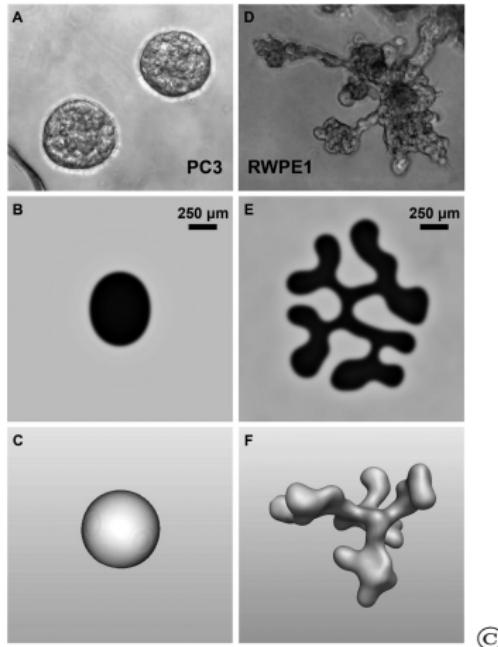
Topology optimization in engineering systems



* 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



G. Lorenzo et al. *Tissue-scale, personalized modeling and simulation of prostate cancer growth*.

Proceedings of the National Academy of Sciences of the United States of America,
113: E7663–E7671, 2016.

Remarks on CSE

Some perspectives and challenges on CSE

Perspectives:

- Development of increasingly realistic models
- Frequent use outside engineering

Challenges:

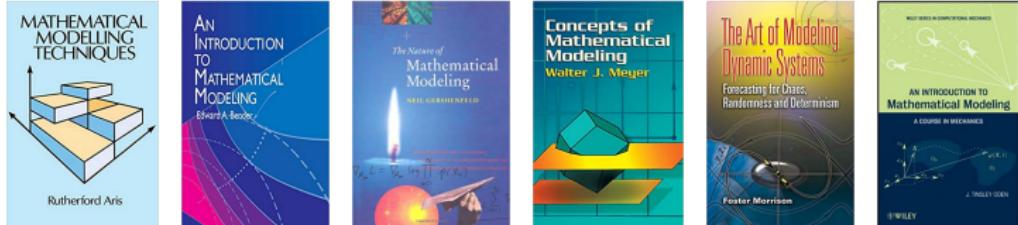
- Data-driven methods to construct high-fidelity models
- Strict procedures for verification of computational codes
- Suitable frameworks for validation of models
- Hardware, software and algorithms for extreme-scale computing

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