Simulation, Analysis, and Validation of Computational Models

— Simulation projects (Case Studies IV) —

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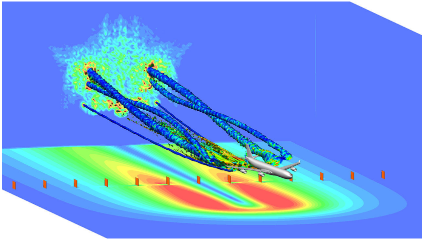
Case studies

- C1: Robot simulators
- C2: Financial markets
- C3: Weather and climate
- C4: Modelling and simulation projects

Ten Phases of a Simulation Project

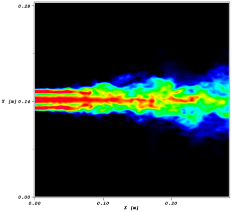
1. Identify problem
2. Acquire background information
3. Formulate problem
4. Decide model type
5. Specify model based on data
6. Code simulation
7. Verify model by tests
8. Document performance, limitations, help files
9. Implementation with stakeholders
10. Validation, maintenance, updates



A. G. Greenwood (2020) A specification for effective simulation project management. WSC, p. 2482.
Discusses 5 phases, namely initiation, planning, execution, monitoring and controlling, and closing.

Simplified procedure

- Given (What is known?)
- Desired (What ought to be done?)



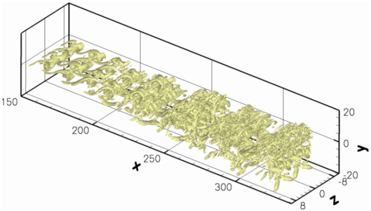
Why are any available approaches/methods/tools insufficient?

- Cost, resources: ⇒ Funding, investment, propaganda
- Skills, background, knowledge ⇒ Training, consulting
- Improvement needed ⇒ Optimisation, machine learning
- Fundamental limitations ⇒ Research, experimentation

What is known?

- Variables
- Parameters
- Time scales
- Length scales
- Interactions
- Dynamics
- Noise
- Local expert knowledge
- State of the art
- Rules and regulations
- Responsibilities

- Data availability



What ought to be done?

Change open questions to answerable questions w.r.t. a goal:

- What should be known?
- What can be found out?
- What can be changed?
- What risks exist?
- What can be excluded?
- What can happen?
- Is it possible to ...?
- How quickly?
- At what cost?
- Can the *goal* be achieved more robustly?
- Can the *goal* be achieved more economically?

Practical approach

Get a solid background on the problem $\Leftrightarrow$ Discuss with experts and stakeholders

Consider now a few examples ...

D. Dörner: "The Logic of Failure" (1989)

Recognizing And Avoiding Error In Complex Situations

Departing from our topic for a moment, we consider here the use of computer simulations of complex systems as a tool to learn about *mental simulations* in humans

- Human psychology in a (simulated) complex world
- Use good funding to improve the situation of the people in rural "*Tanaland*" during 10 years of simulated real time
- Control in this simulation has side effects and changes occur being caused by the player only indirectly.

Similar scenarios (all in simulations):

- Govern as small town
- Maximise the profit of a company
- Control the temperature of a refrigerated warehouse

D. Dörner: "The Logic of Failure" (1989)
Recognizing And Avoiding Error In Complex Situations

Only a minority of participants did well (uncorrelated to intelligence)

What they were doing right:

- Define a clear (preliminary) goal to be able to evaluate the situation
- Use initially a model sketch and improve it continually
- Do not stop to collect information
- Prognosis and extrapolation help to understand cause and effect
- Plan ahead and make decision early
- Check effect of actions

What were typical errors:

- Choosing false certainty over factual uncertainty
- Dwindling information acquisition
- Complex systems are hard to understand, so don't try
- Waiting for things to "break" before acting
- Ignore "distractions" outside current focus
- Avoid errors at all cost

A simple feedback system

Task:	Tell what is going to happen
Given:	Current state, interactions
Need:	Prediction
Goal:	Correct prediction
Validation:	Check in real system

Simulation can use differential equations or maps and results typically in a critical revision of the system $\rightarrow$ better understanding of the system

Example "Motivational state"

$S(t)$ motivational state of self at time t
$O(t)$ motivational state of others at time t

$$\dot{S}(t) = a\,S + b\,O$$

$a, b > 0$: eager
$a, b < 0$: negative
$a < 0, b > 0$: cautious
$a > 0, b < 0$: narcissistic

Linear equations can imply exponential grow, therefore

- Set hard limits (if $S > 1$ then $S = 1$)
- Set soft limits
  - in maps: $S_t = \mathrm{sigmoid}(f(S_{t-1}))$
- Use self-limiting dynamics
  - in systems: $\dot{S} = (a\,S + b\,O)(1 - S)$ or $\dot{S} = (a\,S + b\,O) - S^3$

S.H. Strogatz (1988) Love affairs and differential equations. Mathematics Magazine 61:35.

"Love affairs and differential equations"

Original Romeo is excited by the love experienced from Juliet.
Juliet enjoys own feelings, but disapproves Romeo's advances.

$$\begin{aligned} \dot{R}(t) &= J \\ \dot{J}(t) &= J - R \end{aligned}$$

$$\begin{aligned} \dot{R}(t) &= aJ \\ \dot{J}(t) &= bR \end{aligned}$$

Matrix $\begin{pmatrix} 0 & a \\ b & 0 \end{pmatrix}$, eigenvalues $\lambda_{1/2} = \pm\sqrt{ab}$ ($\det = -ba$, $\mathrm{Tr} = 0$)

$a \cdot b > 0$, eigenvalues real: saddle point, emotions tend to $\left(1, \sqrt{\frac{b}{a}}\right)$

$a \cdot b < 0$, eigenvalues imaginary: carousel of emotions

S.H. Strogatz (1988) Love affairs and differential equations. Mathematics Magazine 61:35.

Do opposites attract?

$$\begin{aligned}\dot{R}(t) &= aR + bJ \\ \dot{J}(t) &= -bR - aJ\end{aligned}$$

Matrix $\begin{pmatrix} a & b \\ -b & -a \end{pmatrix}$, eigenvalues $\lambda_{1/2} = \pm\sqrt{a^2 - b^2}$

($\det = b^2 - a^2$, $\mathrm{Tr} = 0$) $a > b$ saddle, $a < b$ spirals

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$$\begin{aligned}\dot{R}(t) &= aR + bJ \\ \dot{J}(t) &= bR + aJ\end{aligned}$$

Matrix $\begin{pmatrix} a & b \\ b & a \end{pmatrix}$, eigenvalues $\lambda_{1/2} = a \pm b$ ($\det = a^2 - b^2$, $\mathrm{Tr} = 2a$)

$a > b > 0$, eigenvalues real: emotions continue to grow

$a < b$, saddle point, emotions tend to $(1, 1)$

S.H. Strogatz (1988) Love affairs and differential equations. Mathematics Magazine 61:35.

Pandemics

Task: Mitigate effects of the disease

Given: Counts of incidents $\rightarrow$ determine rates

Need: Prediction based on an explainable model

Goal: Reduce peak

Simulation can verify goal, test effects of changed rates, measurement intervals, role of delays (incubation) and noise, and side effects to economy, safety and well-being

- Susceptible, Infectious, or Recovered
- Rates: Infection α, recovery β (w/o immunity), γ (w/ immunity)
- Normalisation $R(t) + S(t) + I(t) = 1$ conserved by balanced equations (i.e. already two equation would be sufficient)

$$
\begin{aligned}
S(t+1) &= S(t) - \alpha S(t)\, I(t) + \beta I(t) \\
I(t+1) &= I(t) + \alpha S(t)\, I(t) - \beta I(t) - \gamma I(t) \\
R(t+1) &= R(t) + \gamma I(t)
\end{aligned}
$$

- Include also vaccination rate μ (SIRV)

$$
\begin{aligned}
S(t+1) &= S(t) - \alpha S(t)\, I(t) + \beta I(t) - \mu S(t) \\
I(t+1) &= I(t) + \alpha S(t)\, I(t) - \beta I(t) - \gamma I(t) \\
R(t+1) &= R(t) + \gamma I(t) + \mu S(t)
\end{aligned}
$$

Susceptible, Infectious, or Recovered ($\beta = 0$, $\gamma + \beta \to \gamma$)

$$\dot{S} = -\alpha\, I\, S - \mu\, S$$

$$\dot{I} = \alpha\, I\, S - \gamma\, I$$

$$\dot{R} = \gamma\, I + \mu\, S$$

Low level simulation (compare large-scale simulation)

- Task: Provide decision support
- Given: Incidences, rates
- Need: Prediction of effect of changed rates
- Goal: Keep peak low
- Validation: Check changes of incidences

Economical processes

Task: Decision making (e.g. market introduction)

Given: Data, elasticities (more supply can decrease price)

Need: Conditional prediction based on model

Goal: Find strategies for campaigns, pricing, presentation

Simulation can

- predict effect of action
- check elasticity values based on data
- identify market heterogeneity

Robot control

Task: Move closer to goal

Given: Sensor values $\rightarrow$ direction to goal

Need: Motor action to reach goal $\rightarrow$ determine Jacobian to find required change in motor space

Goal: Arrive at goal

Validation: Check for decrease of distance to goal

Simulation can verify goal by extracting information from sensors, determining update intervals, analysing stability, role of delays and noise, and side effects

"High-level" robot control

Task: Motion planning

Given: Sensor values $\rightarrow$ direction to final goal

Need: Foot placement $\rightarrow$ Specify subgoal (integer optimisation + within–step control)

Goal: Arrive at final goal

Validation: Check for decrease of distance to goal

Simulation can verify goal by extracting information from sensors, determining update intervals, analysing stability, role of delays and noise, and side effects from low-level processes, cross-torque from other degrees of freedom, and react and anticipate to effects from environment, optimise energy consumption, wear, and risk

Climate control

Task: Decision making

Given: Data

Need: Conditional prediction based on model

Goal: Estimate effect of action

Simulation can

- predict effect of action
- check consistency of data based on model assumptions (and thus validity of model)

Conclusion on simulations

- Simulation depends on domain knowledge and on available information
- Ambiguity of data uncertainty and model uncertainty
- Improving model can be easier than getting better data

A brief look at high-performance computing

Implied by

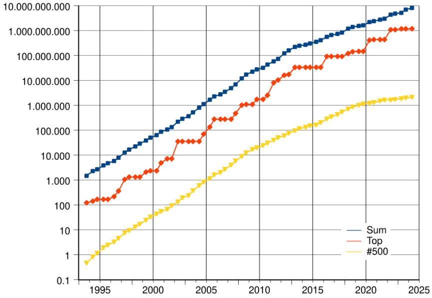
- High degree of realism
- Need for strong risk reduction
- Difficult learning tasks,
- Large sets of agents
- Complex materials and environments
- Challenging simulations

High-performance computing: Applications

- Cryptanalysis
- Weather forecasting, climate research,
- Physics :
  - Modelling the early universe, black holes
  - Quantum mechanics
  - Structure and properties of chemical compounds and biological macromolecules, polymers, crystals
  - Identifying the spike protein in the COVID-19 virus
- Energy
  - Oil and gas exploration
  - Nuclear fusion
- Military: detonation of nuclear weapons
- Engineering: airplane and spacecraft aerodynamics,

High-performance computing

- Folding@home: 2.43 exaflops by April 12, 2020
- Exascale computing: HPE Gray EX
- 100,000 GPU AI cluster — xAI Colossus



T top 500 (total), Current #1, Current #500 (GFLOPS)
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Conclusion

- Simulation can run at and connect several levels of description
- Discussion of learning vs. modelling is on-going
- Explainability, energy consumption and accessibility is key

Remaining topics

12 Modeling and simulation and explainability (week 8/2)

B1 PINN (week 6/2)

B2 More on PINNs (week 9/1)

B3 Industry 4.0 (week 9/2)

B4 Digital twins (week 10/1)

R Revision (week 10/2)