Numerical Modelling
- Introductory Approach

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Jérôme Frisch
Technische Universität München
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Why do we need numerical simulation

- why numerical simulation?
  - because experiments are sometimes *impossible*
    - life cycle of galaxies, weather forecast, terror attacks, e. g.
  - because experiments are sometimes *not welcome*
    - avalanches, nuclear tests, medicine, e. g.
Why do we need numerical simulation

- why numerical simulation? (cont’d)
  - because experiments are sometimes *very costly and-time consuming*
    - protein folding, material sciences, e. g.

- because experiments are sometimes *more expensive*
  - aerodynamics, crash test, e. g.
Overview - The Main Elements of Simulation

Physical System → Mathematical Model → Simulation → Prediction

Validation: Do we solve the right mathematical model?

Verification: Do we solve the mathematical model correctly?
Types of Models

- Physical Models / Models of natural science
  
  "Scale representation of physical phenomena"

  - image of nature, highlighting essential properties
  - mainly based on hypotheses (= model), illustration of phenomena
  - "Exact Science", low level of abstraction

- Mathematical Models
  
  "Description of physical behavior with predefined formalism"

  - image of systems / natural phenomena
  - based on models from natural science (physics, chemistry, biology, ...) or similar

- Engineering Models
  
  "Physical and mathematical model on a higher abstraction level"

  - often simplified approach → restriction to essential system behavior
  - well suited for analyses and simulation
Principles of Mathematical Modelling

- Description of a given problem with **mathematical formalism** in order to
  - get a formal and precise description (e.g. PDE)
  - uncover essential properties and behavior due to abstraction
  - allow systematic analyses i.e. problem solution

- **Modeling** of real system behavior with
  - suitable mathematical formalism (logic, algebraic structures, topology, …)
  - simplification and abstraction in order to reduce complexity

- **Evidence** of model behavior in order to proof real system behavior, e.g. in
  - exact natural science and engineering (e.g. basic conservation laws of continuum mechanics (energy, mass, momentum, …) → long tradition
  - economics (e.g. law of supply & demand), climate modelling (e.g. interaction of atmosphere, oceans, …)

- Still to do:  **derivation** and **analysis** of models
Derivation of Models

- **Purpose of the modelling**
  - What has to be analysed? → stability or serviceability of a structure
  → motion of a single person or of a crowd

- **Input parameter**
  - What are the important quantities?
    → Optimum trajectory of the space shuttle: gravitation of Earth or Pluto?
    → Climate change: what are the lasting effects of wildfire?
    → Oscillation of a bridge: excitation frequency or load participation or both?
Derivation of Models

- **Purpose of the modelling**
  - What has to be analysed?

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  - What are the important quantities?

- How do these parameters influence the model behavior?

- How do these parameters behave?
Derivation of Models

- **Purpose of the modeling**
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  - How do these parameters influence the model behavior?
    - May we neglect some of them? (Neglect damping in oscill. problems?)
    - How well are they determined? (good laboratory values, empirical values?)

  - How do these parameters behave?
    - Qualitative/quantitative behavior: Individual character stronger than group dynamics?
Derivation of Models

- **Mathematical description**
  - Differential equations (equilibrium conditions of differential subsystems)
    typical engineering approach for e.g.
    - heat flow
    - elasticity, ...
  - Variational formulation (extreme values of a functional)
    typical approach in natural science for e.g.
    - elasticity, ...
  - Relational algebra / Graph Theory / Automata
    - shortest path problem
    - critical path problem
    - capacity problems
    - spread of wildfire
    - crowd behavior
    ...

Types of Analyses

- **Elasticity analysis**
  
  Find the critical behavior:
  Deflection under snow loading?

- **Flow field analysis**
  
  Find a solution:
  Well-being in offices?
Types of Analyses

- Air flow simulation

  temperature distribution?
  comfort behavior?
Types of Analyses

- **Path algebra** →

  - Shortest path (time, distance)?
  - Most reliable path?
  - Is there a Eulerian path?

- **State Transition** →

  - How do crowds behave?
Properties of Models

- What can be said about the solution?
  - **Existance** of a solution

\[ A \mathbf{x} = \mathbf{b} : \quad \text{rank}[A, \mathbf{b}] > \text{rank}[A] \quad \Rightarrow \quad \text{no solution!} \]
Properties of Models

- What can be said about the solution?
  - Existence of a solution
    - Eulerian Path (Königsberg Bridge Problem, Euler 1736)
    - number of vertices with odd vertex degree > 2 \( \Rightarrow \) no solution!
Properties of Models

- What can be said about the solution?
  - **Existence** of a solution
  - **Uniqueness** of a solution

\[ A \mathbf{x} = \mathbf{b} : \quad \text{rank} [\mathbf{A}, \mathbf{b}] = \text{rank} [\mathbf{A}] < N \implies \text{arbitrary solutions!} \]
Properties of Models

What can be said about the solution?

- **Existence** of a solution
- **Uniqueness** of a solution

Fastest connection?  Most reliable path?  Shortest path?
Properties of Models

- What can be said about the solution?
  - Existence of a solution
  - Uniqueness of a solution
  - Dependency on the input data

  - Load distribution, e.g. on structures
  - Number of load cases
  - Effects of ad-hoc decisions (choice of a start iteration vector, subspace size, …)
  - Influence of experimental input data (material law, …)
  - Influence of empirical input data (sociological aspects, …)
Properties of Models

- What can be said about the solution?
  - **Existence** of a solution
  - **Uniqueness** of a solution
  - **Dependency** on the input data

- What can be said about the solution method?
  - Is the derived model suited for a numerical solution strategy (granularity) ?
  - Well-transformable to a suitable system of equations (simplifications) ?
  - How much is the solution method dependent on human intelligence (experience/professional background) ?

- What about correctness of the derived model?
  - Degree of abstraction? Still a realistic model?
  - Do validation methods exist? Is experimental validation feasible?
Solution approach

- **Analytical** solutions
  - Highly desired, not always possible
  - Formal proof of existence and uniqueness of a solution

- **Heuristic** solutions
  - Trial and error, following some solution strategy („search methods“)
  - Well-suited e.g. for travelling salesman problem (logistics, machine control,…)
  - Also used for root finding for polynomials and optimization

- **Numerical** solutions
  - Direct solution (Simplex(Optimization), LU-decomposition, …)
    - partially exact solution possible
  - Iterative solution (Jacobi, CG, QR, Gauß-Seidel, GMRES, …)
    - approximation of exact solution!
Questions?