What is Scientific Computing?

- mathematical and informatical basis of numerical simulation
- reconstruction or prediction of phenomena and processes, esp. from science and engineering, on supercomputers
- third way to obtain knowledge apart from theory and experiment

transdisciplinary: mathematics + informatics + field of application!!

Objectives depend on concrete task of simulation:
- reconstruct and understand known scenarios (natural disasters)
- optimize known scenarios (technical processes)
- predict unknown scenarios (weather, new materials)

What’s in a Name?

- scientific computing?
- scientific and engineering computing?
- computational science and engineering?
- simulation?

A chemist’s provoking question:

What the hell is non-scientific computing?

The scientific computer’s answer:

What you do, for example! 😊
Why Numerical Simulations?

- since experiments are sometimes impossible:
  - astrophysics: life cycle of galaxies etc.
  - geophysics: displacement of the earth’s magnetic field
Why Numerical Simulations?

- since experiments are sometimes impossible:
  - astrophysics: life cycle of galaxies etc.
  - geophysics: displacement of the earth's magnetic field
  - climate research: Gulf Stream, greenhouse effect etc.
  - weather forecast: tornadoes – where, when, and how strong?
  - security: 1993 bomb attack in the World Trade Center
Why Numerical Simulations?

- since experiments are sometimes impossible:
  - astrophysics: life cycle of galaxies etc.
  - geophysics: displacement of the earth's magnetic field
  - climate research: Gulf Stream, greenhouse effect etc.
  - weather forecast: tornadoes – where, when, and how strong?
  - security: 1993 bomb attack in the World Trade Center
  - propagation of harmful substances
  - economics: development of the stock market etc.
  - medicine: adaptive materials in implants

Why Numerical Simulations?

- since experiments are sometimes very unwelcome:
  - the bad guy: tests of nuclear weapons
  - statics: stability of buildings etc.
Why Numerical Simulations?

➢ since experiments are sometimes rather unwelcome:
  • natural disasters: avalanches

➢ security: effects of car bombs
Why Numerical Simulations?

➢ since experiments are sometimes extremely costly:
  • influence of radiation on the genetic makeup
  • analysis and study of proteins
  • molecular dynamics and behavior of molecules

Why Numerical Simulations?

➢ since simulations are sometimes just cheaper or faster, resp.:
  • aerodynamics, turbulence: objects in a wind tunnel and so on

Re = 3000
Why Numerical Simulations?

- since simulations are sometimes just cheaper or faster, resp.:
  - aerodynamics, turbulence: objects in a wind tunnel and so on

Why Numerical Simulations?

- since simulations are sometimes just cheaper or faster, resp.:
  - aerodynamics, turbulence: objects in a wind tunnel and so on
  - process engineering: mixing processes
  - car industry: crash tests
  - car industry: 65 km/h
US Government: Grand Challenges

- climate research
- combustion
- automobile development
- aircraft design
- electronic design automation
- biology and medicine
- chemistry and physics
- material science
- financial engineering
- ...

From Phenomena to Predictions

- phenomenon, process etc.
  - mathematical model
    - numerical algorithm
      - simulation code
        - results to interpret
          - modelling
          - numerical treatment
          - implementation
          - visualization
          - embedding

- validation
  - statement
  - tool
Mathematical Modelling

- model as a (simplifying) formal abstraction of reality
- issues when deriving a mathematical model:
  - Which quantities have some influence, and how important is it?
  - What relations exist between them? "Which type of mathematics?"
  - What is the given task (solve, optimize, etc.)?
- issues when analyzing a mathematical model:
  - What can be said about existence and uniqueness of solutions?
  - Do the results depend continuously on the input data?
  - How accurate is the model, what can be represented?
  - Is the model well-suited for a numerical treatment?
- There is not one correct model, but several possible!
- model hierarchy: accuracy vs. complexity
- example: simulations concerning man

Simulating Men: Levels of Point of View

<table>
<thead>
<tr>
<th>issue</th>
<th>level of resolution</th>
<th>model basis (e.g.!)</th>
</tr>
</thead>
<tbody>
<tr>
<td>global increase in population</td>
<td>countries, regions</td>
<td>population dynamics</td>
</tr>
<tr>
<td>local increase in population</td>
<td>villages, individuals</td>
<td>population dynamics</td>
</tr>
<tr>
<td>man</td>
<td>circulations, organs</td>
<td>system simulator</td>
</tr>
<tr>
<td>blood circulation</td>
<td>pump/channels/valves</td>
<td>network simulator</td>
</tr>
<tr>
<td>heart</td>
<td>blood cells</td>
<td>continuum</td>
</tr>
<tr>
<td>cell</td>
<td>macro molecules</td>
<td>continuum</td>
</tr>
<tr>
<td>macro molecules</td>
<td>atoms</td>
<td>molecular dynamics</td>
</tr>
<tr>
<td>atoms</td>
<td>electrons or finer</td>
<td>quantum mechanics</td>
</tr>
</tbody>
</table>
What else has to be done?

- in practice, models can typically not be solved \textit{analytically}
- \textit{numerical} (approximate and computer-based) methods!
- the numerical part is non-trivial:
  - often complicated geometries (seeping processes in soil)
  - often changing geometries (a sail in the wind)
  - accuracy requirements force a high resolution of the domain
  - also higher dimensional problems:
    - quantum mechanics: $d=6, 9, 12, \ldots$; finance: $d=365$
  - time dependence (unsteady phenomena)
  - high memory requirements
  - often poor convergence of standard methods (long run times)
  - multiscale phenomena (turbulent flows)

Numerical Treatment of Models

- many approximations and compromises:
  - \textit{numbers}: fixed number of digits instead of real numbers
  - \textit{functions}: approximating polynomials instead of series
  - \textit{domains}: polygonally bounded, restriction to grid points
  - \textit{operators}: difference quotients instead of derivatives
  - \textit{function spaces}: only finite-dimensional
- requirements to be fulfilled by numerical algorithms:
  - \textit{efficient}: high accuracy with moderate storage investment
  - \textit{fast}: the approximate solution is computed in short time
  - \textit{stable}: no significant/qualitative errors in the results
  - \textit{robust}: can be applied for a large class of problems
- main tasks:
  - \textit{derive} the discretized equations
  - \textit{solve} the resulting discrete system of equations
What else has to be done?

- A numerical algorithm is not yet an efficient code.
- The implementation is crucial:
  - Platform microprocessor: pipelining, cache memory.
  - Suitable data structures and organization principles (hierarchy, recurrences).
  - Potential of (automated) parallelization, communication.
  - Today: software engineering important in simulation context, too.
- "MATLAB-numerics" is not sufficient for doing relevant numerical simulations!
- We need "plug-and-play tools": embedding.
- Interpretation of tons of data requires visualization.

---

Literature

- Krabs: *Mathematische Modellierung*, Teubner, `97
- Dongarra et al.: *Numerical Linear Algebra for High Performance Computers*, SIAM, `98
- Griebel et al.: *Numerical Simulation in Fluid Dynamics*, SIAM, `98