Scientific Computing I

Module 1: Introduction

Michael Bader
Winter 2012/2013
Scientific Computing =

Science + Computing?
Scientific Computing =

Science + Computing?

Science on Computers??
Scientific Computing =

Science + Computing?

Science on Computers??

“Computational Science”???
A Short Look into Wikipedia . . .

**Computational science** (or **scientific computing**) is the field of study concerned with

- constructing mathematical models
- and quantitative analysis techniques
- and using computers

To analyze and solve scientific, social scientific and engineering problems.

[...] The scientific computing approach is to **gain understanding**, mainly through the analysis of mathematical models implemented on computers.

[...] Massive amounts of calculations (usually floating-point) and are often executed on **supercomputers** or distributed computing platforms.

[Wikipedia, Sep 21, 2011]
Part I: An Interdisciplinary Discipline

Gaining Scientific Knowledge
The classical scientific process
Approaches to science

The Third Approach – Simulation
Drawbacks of Theory and Experiment
Where Simulation is Needed
Two Large Examples – Astrophysics and Blood Flow
Part II: Tasks of Scientific Computing

The Simulation Pipeline
Stages of the Simulation Pipeline
Disciplines Involved

Roadmap
Part I

An Interdisciplinary Discipline
Gaining Scientific Knowledge

The Classical Scientific Process

1. characterization
   - observation
   - quantification/measurement
Gaining Scientific Knowledge

The Classical Scientific Process

1. characterization
   - observation
   - quantification/measurement

2. hypothesis
   - theory
   - model

Michael Bader: Scientific Computing I
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Gaining Scientific Knowledge

The Classical Scientific Process

1. characterization
   - observation
   - quantification/measurement

2. hypothesis
   - theory
   - model

3. prediction
   - consequences/logical deduction from hypothesis/model?
Gaining Scientific Knowledge

The Classical Scientific Process

1. characterization
   - observation
   - quantification/measurement

2. hypothesis
   - theory
   - model

3. prediction
   - consequences/logical deduction from hypothesis/model?

4. experiment
   - verification/falsification
   - discrepancies might lead to improved model
Gaining Scientific Knowledge (2)

Approaches to Science:

1. theoretical investigation
   - hypothesis / models
   - analytical calculations
   - Gedankenexperiments

2. experimentation
   - build model scenarios
   - predict theoretical results and compare with outcome
Gaining Scientific Knowledge (2)

Approaches to Science:

1. theoretical investigation
   - hypothesis / models
   - analytical calculations
   - Gedankenexperiments

2. experimentation
   - build model scenarios
   - predict theoretical results and compare with outcome

3. simulation
   - *Why would we need that?*
Drawbacks of Theory and Experiment

Theoretical Investigation:

- analytical solutions for simple scenarios, only
- models usually very complicated or even impossible to solve
Drawbacks of Theory and Experiment

Theoretical Investigation:

- analytical solutions for simple scenarios, only
- models usually very complicated or even impossible to solve

Experiments:

- might be impossible to do
- might be dangerous or unwelcome
- might be very expensive
The Scientific Process Revisited

Scientific/Engineering Tasks:

- understand processes (model)
- verify/validate hypotheses/models (experiment)
- design and optimize (model or experiment)
Where Simulation is Needed

Replacing Analytical Solvers:

- analytical solution impossible or hard to compute
- use numerical approximation instead
- application: validate a complex model
  - understand processes
  - validate assumptions
Replacing Experiments:

- analytical theoretical solution available
- replace experiments by simulation of a more detailed model
- application: develop a simple model
  - neglecting non-relevant effects
  - with reduced dimensionality
  - reduced-order models
Where Simulation is Needed (3)

Replacing Analytical Solvers and Experiments:

- detailed and accurate mathematical model given
- use simulation only
- requires real world scenario description
- application: predict reality
  - (weather/climate/earthquake/...) forecasts
  - design and optimization
  - uncertainty quantification
Where Experiments are Impossible

Astrophysics:

- “life cycle” of stars, galaxies, . . .
- motion of planets, asteroids, comets, . . .

Geophysics:

- displacement of the earth’s magnetic field
- continental drift
Where Experiments are Impossible

Meteorology:

- weather forecasts
- simulation of hurricanes and storm surges

Climate and Ocean Modelling:

- greenhouse effect
- ocean currents (gulf stream, etc.)
- tsunami simulation

Image source: Cooperative Institute for Meteorological Satellite Studies, Space Science and Engineering Center, University of Wisconsin-Madison; http://tropic.ssec.wisc.edu/
When There is No Second Try

Stability of Buildings:

- large span bridges or skyscrapers
- consider wind loads, earthquakes, ...

Astronautics

- flight path of space crafts or satellites
- re-entry of space crafts
Where Experiments have Harmful Side-effects

Propagation of Pollutants:

- pollutants in air, water, or soil
- predict long-term behaviour

Nuclear Research:

- security of nuclear power plants
- nuclear weapons
Where Experiments are Expensive

Car Industry:

- aerodynamics
- crash tests
- assembly of parts
- build prototypes or rather simulate?

also combustion processes, vehicle dynamics, ...
Example – Millennium-XXL Project

- $N$-body simulation with $N = 3 \cdot 10^{11}$ “particles”
- compute gravitational forces and effects
  (every “particle” correspond to $\sim 10^9$ suns)
- simulation of the generation of galaxy clusters
  plausibility of the “cold dark matter” model

(Springel, Angulo, et al., 2010)
Example – Millennium-XXL Project (2)

Simulation – HPC-Related Data:

- \( N \)-body simulation with \( N = 3 \times 10^{11} \) “particles”
- 10 TB RAM required only to store particles positions and velocities (single precision)
- total memory requirement: 29 TB
- JuRoPa supercomputer (Jülich)
- simulation on 1536 nodes (each 2x QuadCore, thus 12288 cores)
- hybrid parallelisation: MPI plus OpenMP/Posix threads
- runtime: 9.3 days; 300 CPU years in total

Example – Gordon Bell Prize 2010

(Rahimian, ... , Biros, 2010)

- direct simulation of blood flow
- particulate flow simulation (coupled problem)
- Stokes flow for blood plasma
- red blood cells as immersed, deformable particles
Example – Gordon Bell Prize 2010 (2)

Simulation – HPC-Related Data:

- up to 260 Mio blood cells, up to $9 \times 10^{10}$ unknowns
- fast multipole method to compute Stokes flow (octree-based; octree-level 4–24)
- scalability: 327 CPU-GPU nodes on Keeneland cluster, 200,000 AMD cores on Jaguar (ORNL)
- 0.7 Petaflops/s sustained performance on Jaguar
- extensive use of GEMM routine (matrix multiplication)
- runtime: $\approx 1$ minute per time step

Article for Supercomputing conference:
http://www.cc.gatech.edu/~gbiros/papers/sc10.pdf
Part II

Components of Scientific Computing
The Simulation Pipeline

phenomenon, process etc. → modelling
mathematical model → numerical treatment
numerical algorithm → implementation
simulation code → visualization
results to interpret → embedding
statement tool
Disciplines Involved

- **Mathematics**  
  (modelling, numerics)

- **Computer Science**  
  (implementation, visualization)

- **Engineering & Natural Sciences**  
  (expertise in application area, modelling, validation)
Mathematical Modelling

• classification, types of models
• differential equations
• population models
• heat equations
Numerical Treatment

- discretization
- grid generation, time stepping
- numerical integration of ODE/PDE
- continuous vs. discretized model
Implementation

- data structures and algorithms
- platform-aware programming
- parallel programming
- embedding
Visualization

- visualization techniques
- computational steering
- images first?
Part III

Organisation
Exams, ECTS, Modules

ECTS, Modules
- 5 ECTS (2+2 lectures/tutorials per week)
- CSE: compulsory course
- Biomed. Computing/Computer Science: elective/Master catalogue
- others?

Tutorials:
- tutor: Philipp Neumann
- Mon, 10-12, starting Oct 22

Exam:
- written exam at end of semester
- based on exercises presented in the tutorials