# Ämneskonferens i datavetenskap och numerisk analys, 2006

"Samvaron, numerisk analys och datalogi"

Björn Engquist, CSC. KTH

KTH, Stockholm, 12-14 juni, 2006

#### Overview

- 1. Background: numerical analysis to computational science and engineering
- 2. Relation: numerical analysis computer science
- 3. Comments on teaching

# 1. Background: numerical analysis to computational science and engineering (CSE)

- Computational Science and Engineering Beräkningsvetenskap "The theory and practice of developing and using computations for scientific discovery and engineering applications". Earlier related names:
- Third pillar of science
  - Theory
  - Experiments
  - Computations
- CSE is a general tool and now also enters experiments (compare LHC) and theory (modeling)
- Necessary tool in modern industrial development
- PITAC 2005 report, US gov.
- Towards 2020 Science, Microsoft

#### Driving forces in evolution of NA $\rightarrow$ CSE



NA development and name changes

- Numerical analysis
  - UCLA National Bureau of Standards Institute (≈1950)
  - Development of fundamental concepts in CSE, algorithm, numerical complexity, stability, consistency, iteration, recursion, adaptivity (first golden era: 1945-1980)
  - First pre-computer techniques, interpolation, special functions, etc. then...
  - A new paradigm and new classes of algorithms, CG, QR, MG, FFT, FEM,...

### Computers and Mathematics: Moore's law and numerical algorithms



### NA development and name changes

- Numerical analysis
  - UCLA National Bureau of Standards Institute (≈1950)
  - Development of fundamental concepts in CSE, algorithm, numerical complexity, stability, consistency, iteration, recursion, adaptivity (first golden era)
  - First pre-computer techniques, interpolation, special functions, etc. then...
  - A new paradigm and new classes of algorithms, CG, QR, MG, FFT, FEM,...
- Scientific Computing
  - SIAM Journal (1980s)
  - Stronger coupling to computer development: vector and parallel computing, graphics
  - Some increased awareness of applications

- Computational science and engineering
  - New fields of applications (earlier developed independent of applied mathematics / numerical analysis community)
  - From CFD to material and bio-science, finance, entertainment, environmental, etc.
  - Modeling integrated part of process
  - Many fields of mathematics of importance: probability,...
  - Purpose is scientific discovery and engineering practice
  - CSE core Second golden era ?: 2000-
- Virtual prototyping
  - Industrial CSE
- e-science
  - Stronger coupling to internet
  - Include data intensive and grid computing

"It is the best of times, it is the worst of times"

- Success: CSE has emerged as fundamental in engineering development and scientific discovery. In a remarkable success story the techniques of CSE are rapidly penetrating all fields.
- Problems: CSE (it does not even have an obvious name) is not regarded a scientific field. A victim of its own success: "Everybody is doing it". Is it part of mathematics, computer science or applied fields? Why study - there are standard software systems, etc.

2. Relation: numerical analysis - computer science

- Common origin (1945-55): the computer, programming, the early field of application=science
- Diverging interests (1955-): CS: most applications outside of science, discrete mathematics natural background, "programming" of reduced importance in both CS and NA., few areas of common interest., NA vanishing from CS departments
- Could "broadband" be basis for renewed cooperation?

### Broadband continued

- "Google rather than Microsoft in the future"
- Internet size, bandwidth » infinite dimensions
- Standard graph theory inadequate
- Search engines and SVD
- PDE, harmonic analysis, geometry and statistical techniques dominate modern signal and image processing
- Virtual world of games » virtual prototyping
- Rendering, transformations based on linear algebra and differential equations
- "Physics engines"
- New types of performance oriented systems and hardware, PS3 etc.

#### $\rightarrow$ Shift in focus?

- Continuum mathematics of increased importance (very high dimensions) in particular probability (both NA and CS)
- "Physical" modeling of CS interest
- Hiring of CSE-types in Cs departments
- Hopcroft prediction
- 2020 scienc

### 3. Comments on teaching

- Common problem in CS and NA: rapidly evolving fields new material replacing old
- What to keep of what is in standard software?
- ADB ® Excel
- Linear algebra  $\$  Linpac or  $\$
- Word processing ® Word
- FEM ® Comsol Multi-physics ?
- Teach what is cost effective in a changing world: old principles (the long perspective) and new techniques (skills for the first job some cook-book stuff).
- New alliances: integrated courses (CS-NA, CS/NAapplications, CS/NA-mathematics)
- To lead or to follow "Bologna" an opportunity