DN1240 ht 12
för I

Numeriska metoder

F1

- Översikt 12 F, 6 Ö, X Lab. - följer
- Lärare
  - Davoud Saffar Shamshigar
  - Ludwig Af Klinteberg
  - Jesper Oppelstrup
- Examination
  - 2 Matlab-lab, muntlig redovisning, 1 projekt, skriftlig
  - Tenta – som alla Numme GK (DN1212,1214,…)
    - 1 kryssfrågedel för betyg E
    - 1 med räkneuppgifter

A(n in)convenient truth

It is hard to understand an ocean because it is too big.

It is hard to understand a molecule because it is too small.

It is hard to understand nuclear physics because it is too fast.

It is hard to understand the greenhouse effect because it is too slow.

[Super]Computers break these barriers to understanding. They, in effect, shrink oceans, zoom in on molecules, slow down physics, and fast-forward climates. Clearly a scientist who can see natural phenomena at the right size and the right speed learns more than one who is faced with a blur.

Al Gore, 1990, “Scientific Computing”

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Scientific Computing

Wikipedia:
Scientific computing (or computational science) *is*…
concerned with constructing mathematical models and numerical solution techniques and […] using computers to analyze and solve scientific, social scientific, and engineering problems.

"Numerical analysis is the study of algorithms for the problems of continuous mathematics
[…] to compute quantities that are typically uncomputable,
[…] with lightning speed"
(L.N.Trefethen 1992)

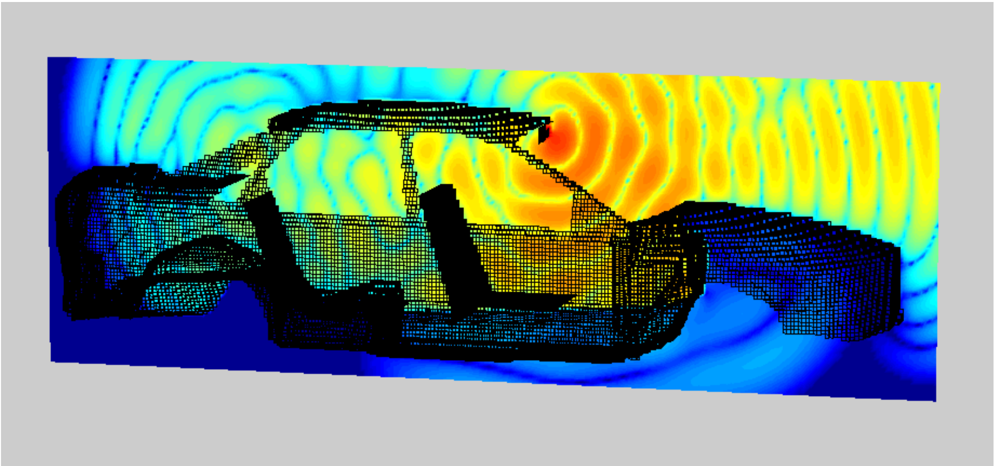
"The purpose of computing is insight, not numbers."
(R.W.Hamming)
***"The Unreasonable Effectiveness of Mathematics"* (1980)**

Computer simulation is … the third paradigm of science

”Simulation has become recognized as the third paradigm of science, the first two being experimentation and theory.”

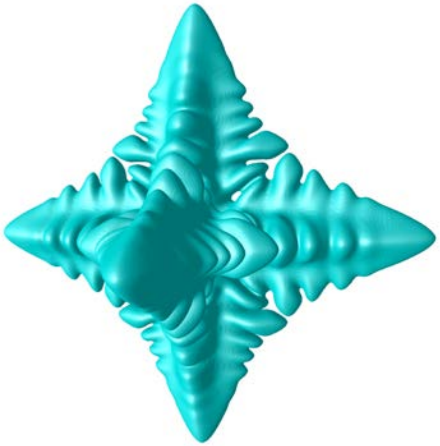
High Performance Computing and Communications:
Foundation for America's Information Future
(Supplement to the President’s FY 1996 Budget)

Antenna in rear-view mirror: Directivity, EMC, …



Maxwell simulator
(T.Rylander & al, CTU)

Dendritic solidification



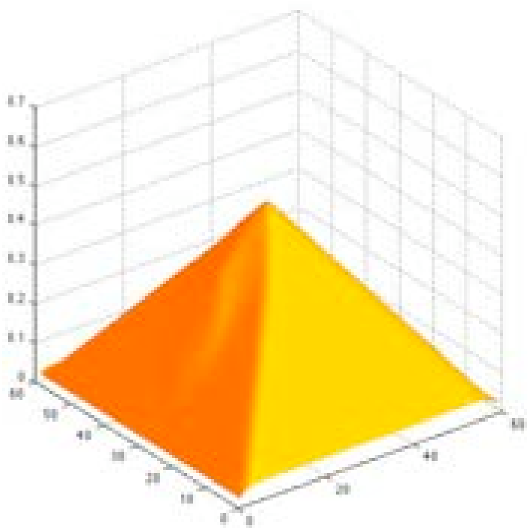
Phase-field simulator

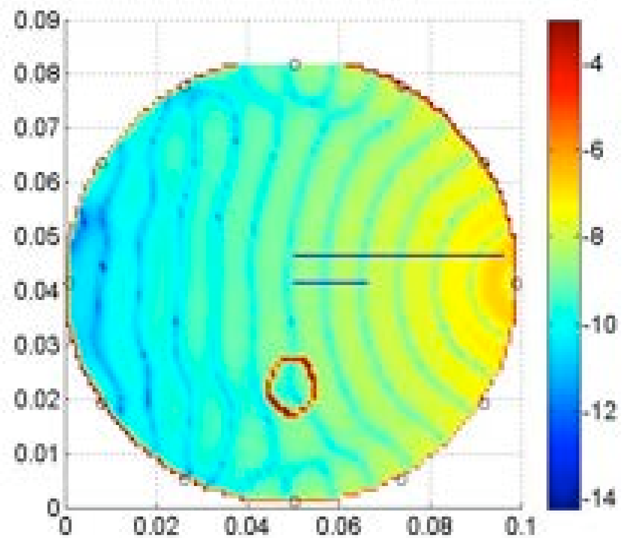
(G.Amberg & al, KTH)

“There are three kinds of lies:
Lies, damn’ lies, and colorful computer pictures” (P.Colella)

Differential Equation Models

Shortest path | Micro-wave tomography | Tsunami





$$\left|\nabla T(x,y)\right| = 1/c(x,y) \text{ in } \Omega, \quad T = 0 \text{ on } \partial\Omega$$

$$\Delta\phi + k^2(a(x,y) + ib(x,y))\phi = 0$$

$$\begin{cases} h_t + hu_x + h_x u = 0 \\ u_t + uu_x + g(h_x + H_x) = 0 \end{cases}$$

Eikonal | Helmholtz | Shallow Water

Computational Materials Science

$$\sigma^{ij}_{,j} = F_i$$

$$\sigma^{ij} = \mu(u^i_{,j} + u^j_{,i}) - \lambda u^k_{,k}\delta^{ij}$$

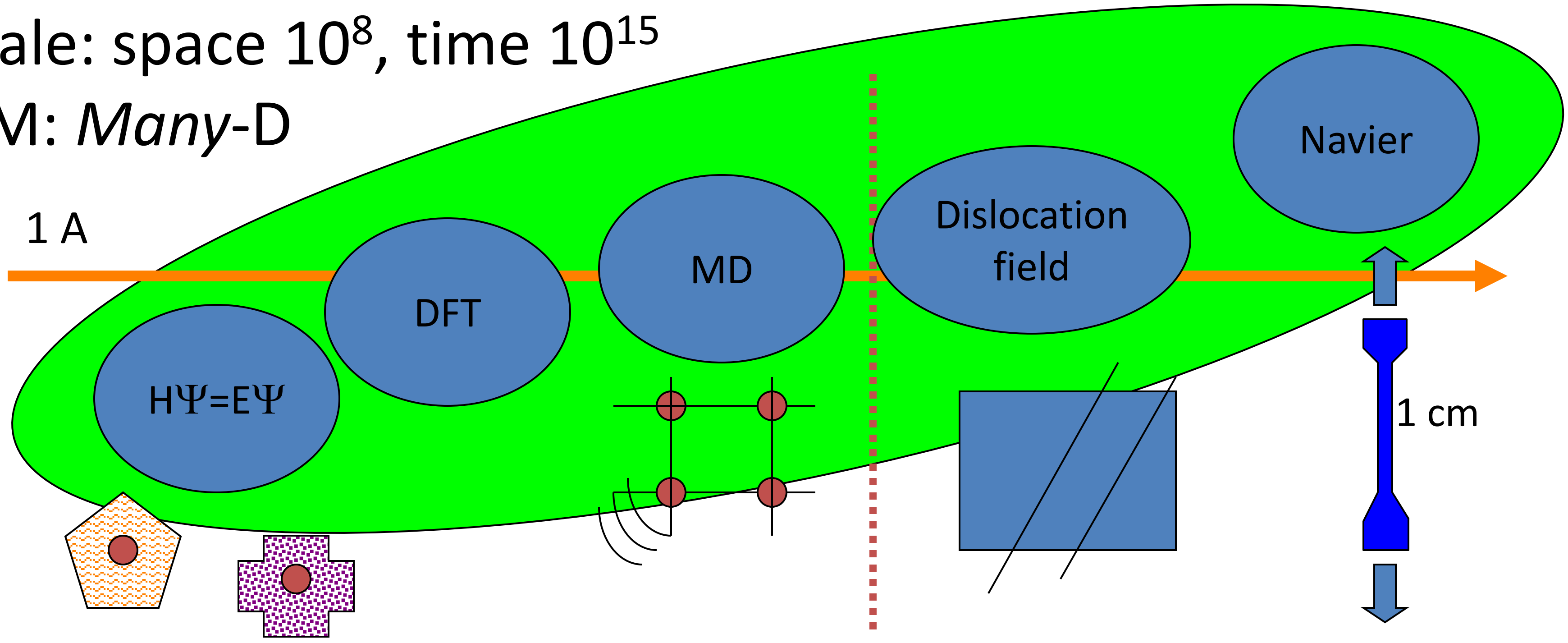
From quantum mechanics to structures:

Goals:

- Predict macroscopic properties from first principles
- Design new materials (ex. nano-technology)

Scale: space 10^8, time 10^{15}

QM: *Many*-D



Success Story I: MATLAB

Major tool for engineering computing,
Numerical analysis, visualization …
1974 “Matrix Laboratory” C.Moler
Now: MathWorks > 1000 pers.
20th anniversary 2005:

Success Story II: comsol

Multiphysics FE software
S.Littmarck
1995: MATLAB PDEToolBox
Now: Comsol > 150 pers.

- “Numerical Methods 101"   2012

1. Why numerical methods? What can be computed?
2. Approximation, iteration, linearization, algorithm
3. Ordinary differential equations:

   simulation, examples

1. Partial differential equations:

   simulation, exempel

Most solutions are approximations!

$$x^2 = 2$$

$$x = \pm\sqrt{2} \approx \pm 1.414$$

Compute … but how?

1. Calculator ... but how does it do it?
2. Mathematics:

$$(1+x)^{1/2} = \sum_{k=0}^{\infty} \binom{1/2}{k} x^k = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \frac{1}{16}x^3 - \frac{5}{128}x^3 + \ldots$$

$$(2)^{1/2} = (\frac{25}{16} + \frac{7}{16})^{1/2} = \frac{5}{4}(1 + \frac{7}{25})^{1/2} =$$

$$= \frac{5}{4}\left(1 + \frac{1}{2}\frac{7}{25} - \frac{1}{8}\left(\frac{7}{25}\right)^2 + \frac{1}{16}\left(\frac{7}{25}\right)^3 - \frac{5}{128}\left(\frac{7}{25}\right)^3 + \ldots\right)$$

$$= 1.25 \times (1 + 0.1400 - 0.0098 + 0.0014 - \ldots) = 1.4145$$

(Puh… despite the convergence acceleration)

Linearisation and ***iteration:*** Newton's method

$$f(x) = 0 : x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, x_0 = \ldots$$

$$f(x) = x^2 - 2 : x_{n+1} = \frac{1}{2}\left(x_n + \frac{2}{x_n}\right)$$

1 1.5 1.417 1.414216 1.4142136

Mmm!

Linjära ekvationssystem

Finn $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ så att $\mathbf{Ax} = \mathbf{b}$, $\mathbf{A} = (a_{ij})$

NAM: 1.4, 1.5, 1.6 (inte 1.6.2), 1.7, 1.8

eller

minstakvadrat-lösning

$\min \|\mathbf{Ax} - \mathbf{b}\|^2$

NAM 2

Olinjär ekvation

Finn x så att $f(x) = 0$

NAM 6

Olinjära ekvations***system***

Finn $\mathbf{x}$ så att $\mathbf{f}(\mathbf{x}) = 0$

NAM 6.8, 6.9

eller

minstakvadrat-lösning

$\min \|\mathbf{f}(\mathbf{x})\|^2$

NAM 6.10

Initialvärdesproblem för ordinära differential-ekvationer

Finn $\mathbf{y}(t)$ för $t > 0$

då $d\mathbf{y}/dt = \mathbf{f}(t,\mathbf{y})$, $\mathbf{y}(0) = \mathbf{c}$

NAM 8.1-8.6

plus extra

Randvärdesproblem för ordinära differential-ekvationer

Finn $\mathbf{y}(x)$ för $a < x < b$

då $d\mathbf{y}/dx = \mathbf{f}(x,\mathbf{y})$,

$\mathbf{G}(\mathbf{y}(a),\mathbf{y}(b)) = \mathbf{0}$

NAM 8.7

plus extra

Partiella differentialekvationer

Initial/randvärdesproblem:

Finn $T(x,t)$ för $0 < x < L$, $t > 0$ då

$$\rho C \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2}; \quad 0 < x < L; t > 0$$

$$T(0,t) = T_0, \quad T(L,t) = T_L$$

$$T(x,0) = f(x)$$

Kvadratur

Beräkna

$$I = \int_a^b f(x)dx$$

$$I = \int_D f(x,y)dxdy$$

NAM 5 Inte 5.2.4,5.2.5;

Optimering

Finn max. för $f(x)$ i

$a < x < b$

NAM 7 (inte 7.1.2)

plus extra

Beräkna $f(x)$ då

$$f(x_i) = y_i, i = 1,2,\ldots,m$$

Interpolation / Approximation

- Tabeller
- Polynom $P_k(x)$
- Spline-funktioner
- Bézier-kurvor

Linjära ekvationssystem

Finn $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ så att $\mathbf{Ax} = \mathbf{b}$, $\mathbf{A} = (a_{ij})$

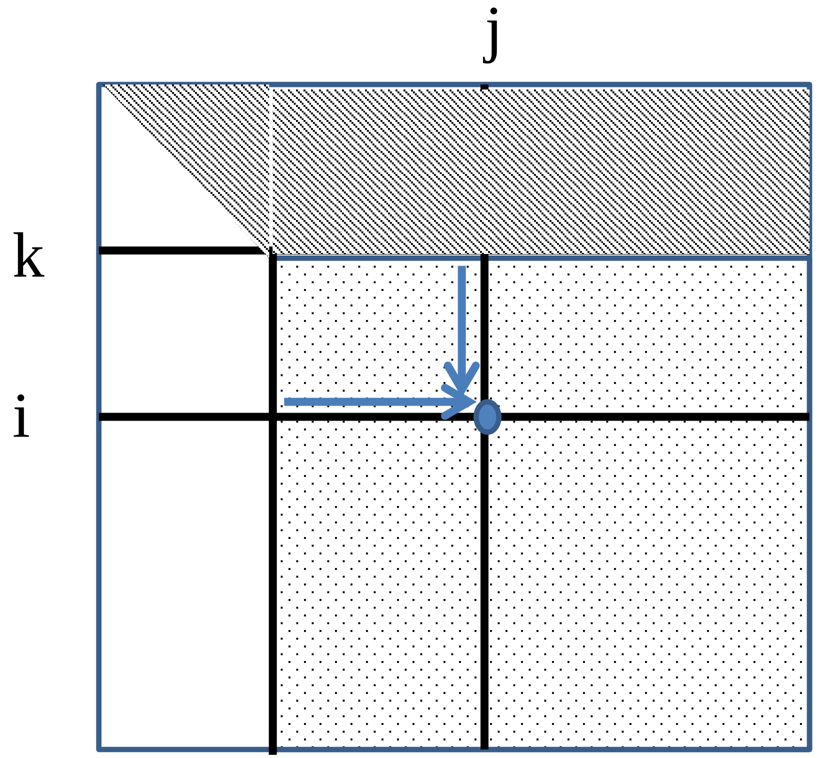
NAM: 1.4, 1.5, 1.6 (inte 1.6.2), 1.7, 1.8

Formulering

Gauss-elimination

Pivotering

Arbetsvolym



Pivot - rad k : för $i = k+1, k+2, \ldots, n$

$$a_{ij} \leftarrow a_{ij} - m_{ik} a_{kj}, \; j = k+1, \ldots, n \qquad m_{ik} = \frac{a_{ik}}{a_{kk}},$$

$$\text{Antal mult. \& add}: \quad \sum_{k=1}^{n-1} (n-k)^2 = \frac{n^3}{3} + O(n^2)$$

Exempel:

Approximation, iteration, linjarisering, algoritm:

Newton-Raphsons metod för lösning av $f(x) = 0$

1. Approximation med ***linjarisering:***

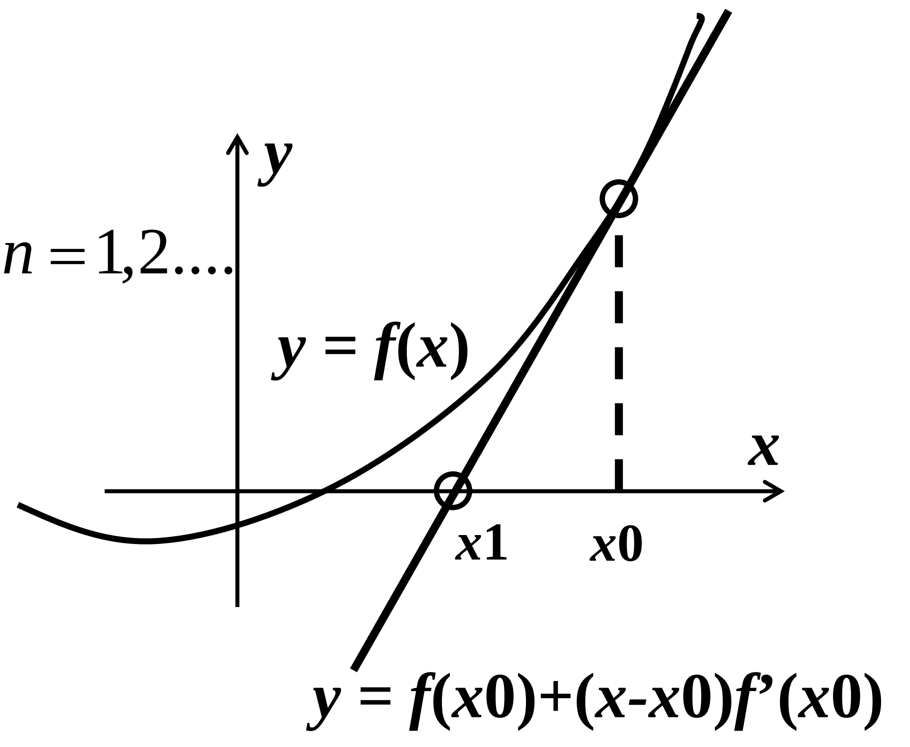
av $y = f(x)$ med tangenten i $(x_0, f(x_0))$,

som har nollställe i

$$x_1 = x_0 - f(x_0)/f'(x_0)$$

2. ***Iteration***: Upprepa!

(*): $x_n = x_{n-1} - f(x_{n-1})/f'(x_{n-1}),\ n = 1,2\ldots$



3. ***Algoritm:***

a) välj x_0 och tolerans ε

b) Iterera med (*) tills

$$|x_n - x_{n-1}| \le \varepsilon$$

c) x_n är närmevärde till nollstället

Exempel

1. Kvadratroten (Herons metod)

$$f(x) = x^2 - 2, \quad f'(x) = 2x:$$

$$x_n = x_{n-1} - \frac{x_{n-1}^2 - 2}{2x_{n-1}} = \ldots = \frac{1}{2}\left(x_{n-1} + \frac{2}{x_{n-1}}\right)$$

2. Division utan divisions-instruktion

Cray – 1, 1976
160 Mflops

$$f(x) = \frac{1}{x} - a \quad f'(x) = -\frac{1}{x^2}:$$

$$x_n = x_{n-1} - \left(\frac{1}{x_{n-1}} - a\right) / \left(-\frac{1}{x_{n-1}^2}\right) = x_{n-1}(2 - ax_{n-1})$$

Division utan division – analys.

$$f(x) = 1/x - a; \; f' = -1/x^2$$

$$x_{n+1} = 2x_n - ax_n^2$$

Vi vill se hur x_n konvergerar mot 1/a och betraktar felet

$$E_n = 1/a - x_n : \ldots$$

$$1/a - x_{n+1} = 1/a - 2x_n + ax_n^2 = a(1/a - x_n)^2 :$$

$$E_{n+1} = aE_n^2$$

med $l_n = \ln E_n$ får vi

$$l_{n+1} = 2l_n + \ln a$$

För tillämpningen på division av binära flyttal är bara ½ < a < 1 intressant, så vi tar a = 1 och l_0 = -1;

$l_n = -2^n$: $\quad E_n = e^{-2^n}$