

DN1215 vt 12 för ME

Numeriska metoder

F1

- Översikt: Lektionsundervisning och dator-laborationer
- Lärare Jesper Oppelstrup
- Examination
 - 2 Matlab-lab, muntlig redovisning, 1 projekt, skriftlig
 - Tenta – som alla Numme GK (1212,1214,...)
 - 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”

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)

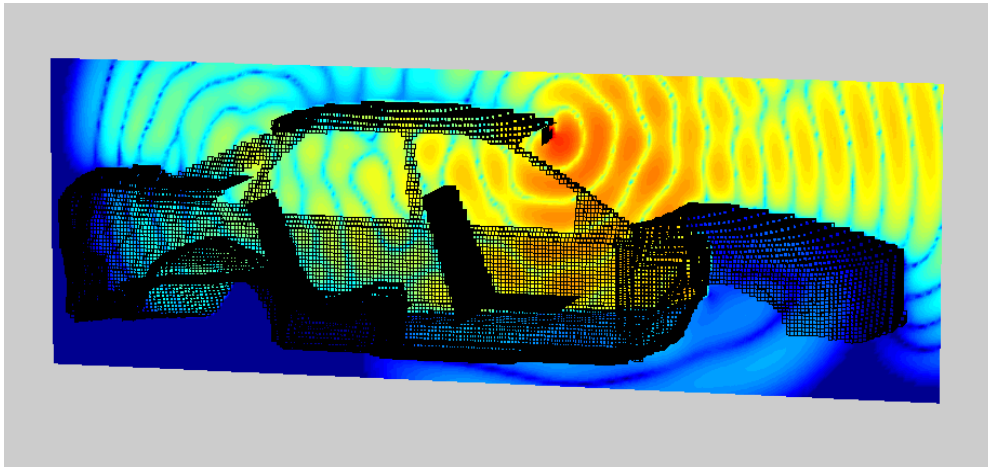


Computer simulation is ... the third paradigm of science

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

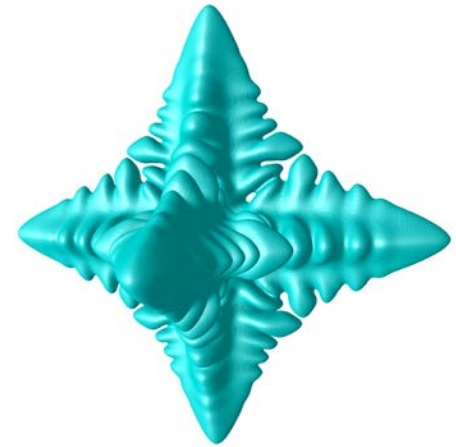
*High Performance Computing and Communications:
Foundation for America's Information Future*
(Supplement to the President's FY 1996 Budget)

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



Maxwell simulator
(T.Rylander & al, CTU)

Dendritic solidification

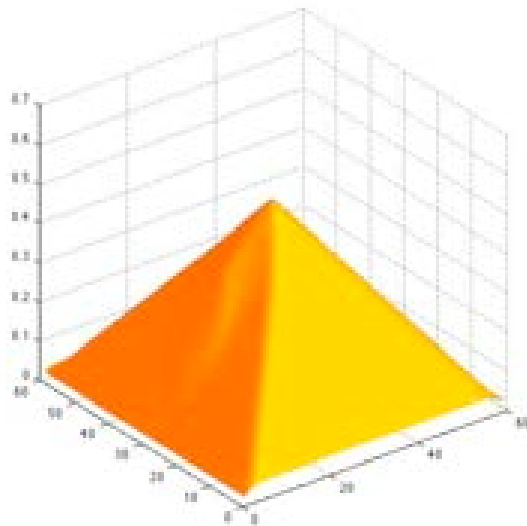


Phase-field simulator
(G.Amberg & al, KTH)

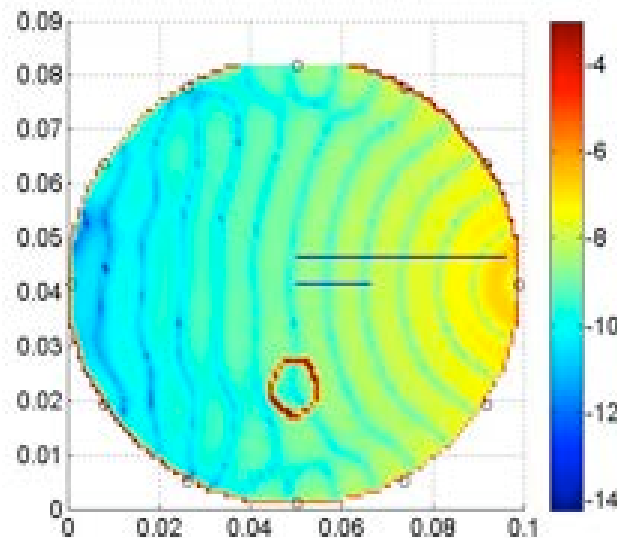
“There are three kinds of lies:
Lies, damn’ lies, and colorful computer
pictures” (P.Colella)

Differential Equation Models

Shortest path



Micro-wave tomography



Tsunami



$$|\nabla T(x,y)| = 1/c(x,y) \text{ in } \Omega, \quad T = 0 \text{ on } \partial\Omega, \quad \Delta\phi + k^2(a(x,y) + ib(x,y))\phi = 0 \begin{cases} h_t + hu_x + h_xu = 0 \\ u_t + uu_x + g(h_x + H_x) = 0 \end{cases}$$

Eikonal

Helmholtz

Shallow Water

Computational Materials Science

From quantum mechanics to structures:

Goals:

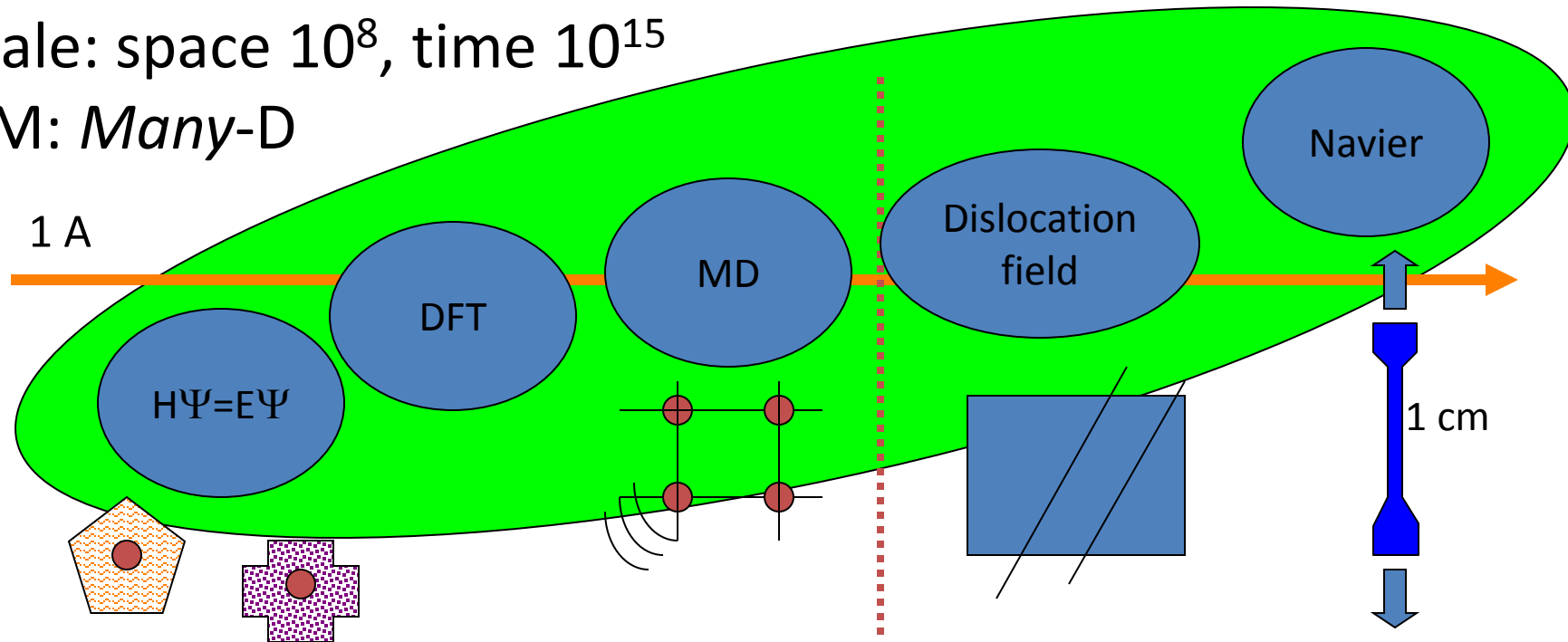
- Predict macroscopic properties from first principles
- Design new materials (ex. nano-technology)

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

QM: *Many-D*

$$\sigma_{,j}^{ij} = F_i$$

$$\sigma^{ij} = \mu(u_{,j}^i + u_{,i}^j) - \lambda u_{,k}^k \delta^{ij}$$



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, example

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:

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

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

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

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

(Puh... despite the convergence acceleration)

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

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

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

1 1.5 1.417 1.414216 1.4142136

Mmm!

Linjära ekvationssystem

Finn $\mathbf{x} = (x_1, x_2, \dots, x_n)$ 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 ekvationssystem

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

Kvadratur

Beräkna

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

$$I = \int_D f(x, y) dx dy$$

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

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

Interpolation / Approximation

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

Linjära ekvationssystem

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

Formulering

Gauss-elimination

Pivoterering

Arbetsvolym

NAM p 7,8

Blandningsproblem:

Råvara R_i ($i=1 \dots n$) har
halterna a_{ij} av

grundpigment j ($j=1 \dots n$)

Hur ska man blanda,

halt x_j av R_j för att få en
produkt med halt w_k av
pigment k ?

$$\mathbf{Ax} = \mathbf{w} : \sum_{j=1}^n a_{ij} x_j = w_i, i = 1, 2, \dots, n$$
$$0 \leq x_j \leq 1$$

MATLAB

% NAMp7 - om färger

lind = [50 20 30 0]';

gras = [30 55 5 10]';

moss = [15 15 45 25]';

hav = [0 10 25 65]';

A = [lind gras moss hav]

wanted = [25 25 25 25]';

x = A\wanted

pause

[50 20 30 0]

- gör radvektor

- ' transponerar till kolumn

A = [lind gras moss hav]

**- gör 4x4 matris genom att
ställa kolumnerna bredvid
varann**

wanted = [25 25 25 25]'

- gör högerled

x = A \ wanted

**- lös med Gauss-elimination
pause**

- stanna

MATLAB

Vilka färger kan blandas?

Simulera! Gör N blandningar där man väljer x_i som positiva slumptal som summerar till 1 ($x_i = \text{halt}$)

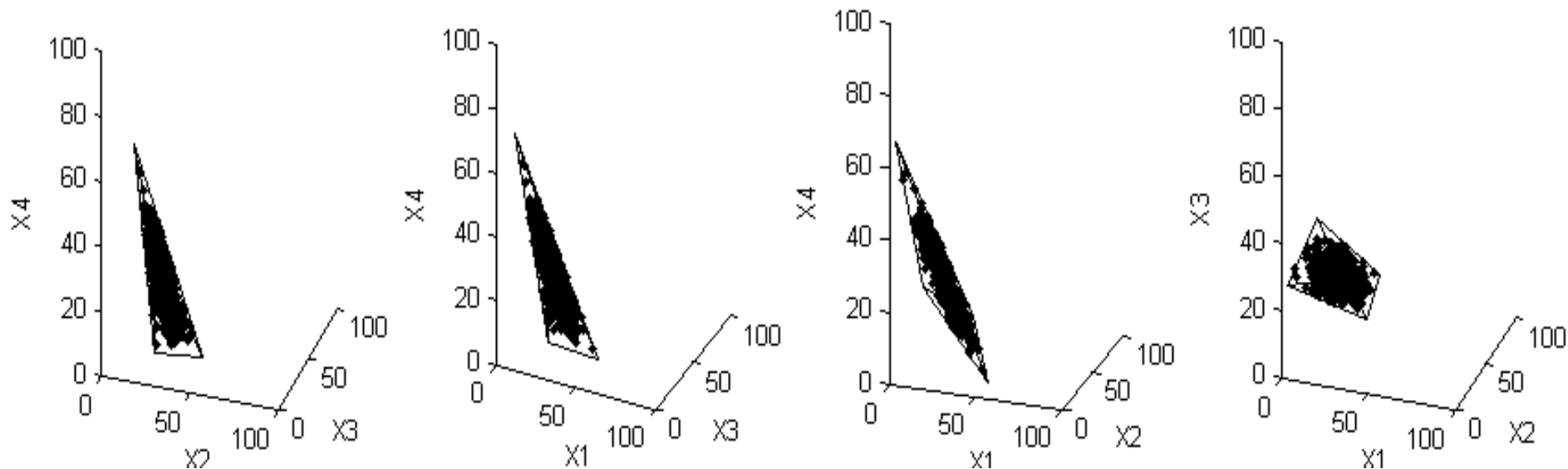
Lagra i en $4 \times N$ tabell $\mathbf{x}$

```
% generera slumptal som summerar till 1;
N = 1000;
x = rand(4,N);    % rand ger slumptal mellan 0 och 1,
                  % 4 rader, N kolonner
s = sum(x,1);      % Summera kolonner
x = x*diag(1./s);  % Dividera kolonn med dess summa
                  % genom multiplikation med diagonalmatris
                  % från höger
y = A*x;           % Blanda!
```

Plotta!

Plotta alla punkterna som ligger i en 4D simplex i $\mathbf{R}^4$ som fyra projektioner på de tre-dimensionella rummen med axlar (x_2, x_3, x_4) , (x_1, x_3, x_4) , (x_1, x_2, x_4) , (x_1, x_2, x_3) :

Alla punkter i projektionerna i 3D simplexar = tetraedrar. Tetraederkanterna plottas.



MATLAB

```
% now plot
axnum = 1:4;
for k = 1:4
    ypl = y;
    ypl(k,:) = [];
    axnumpl = axnum;
    axnumpl(k) = [];
    Apl = A;
    Apl(k,:) = [];
    subplot(1,4,k);
    %clf
    hold on
    plot3(ypl(1,:), ypl(2,:), ypl(3,:), 'k');
    xlabel(['X', num2str(axnumpl(1))])
    ylabel(['X', num2str(axnumpl(2))])
    zlabel(['X', num2str(axnumpl(3))])
    for j = 1:4
        a = Apl(:,j);
        for l = j+1:4
            b = Apl(:,l);
            plot3([a(1),b(1)], [a(2),b(2)], [a(3),b(3)], 'k');
        end
    end
end
axis([0 100 0 100 0 100])
end
```

Plotta i delfönster,
1 rad 4 kolonner, i k:te delfönstret

Plotta i 3D som svarta punkter

Resten av
programmet är
"speciellt";
titta på det
senare

Välj axel-storlek