Numeriska metoder F/CL 2010

Föreläsning 1

Lärare i kursen

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Numeriska metoder?

- Computational Science/Beräkningsvetenskap
- Scientific Computing/Vetenskapliga beräkningar
- High Performance Computing
- Numerisk analys
- Simuleringsteknik
- Beräkningsmatematik

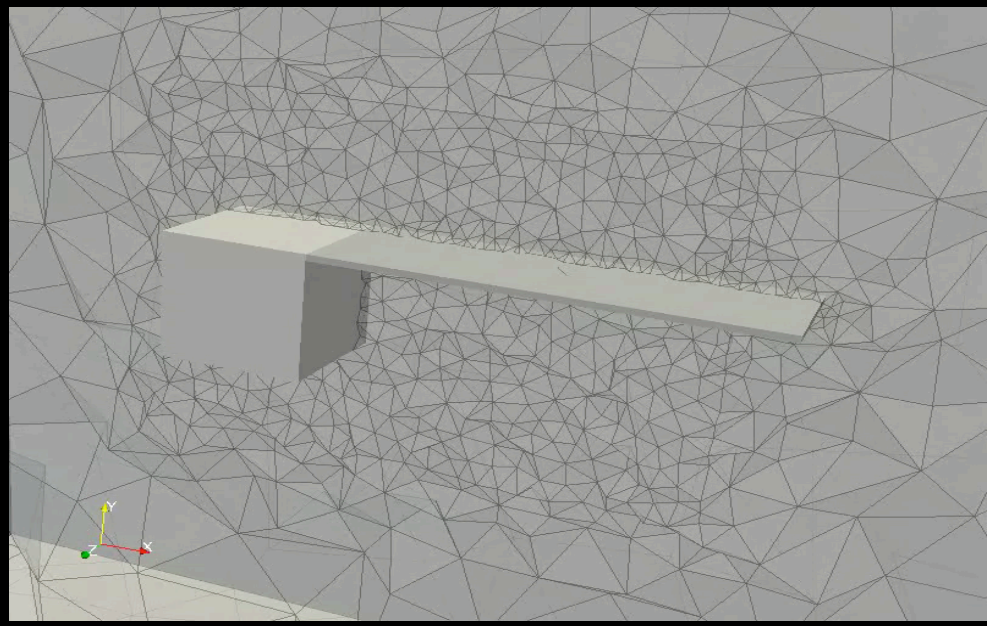
- Matematiska modeller + dator

Modellering och Simulering

- Bygg en matematisk modell (ekvation) av verkligheten
- En ekvation från verkligheten är ofta alltför komplex att lösa med penna och papper

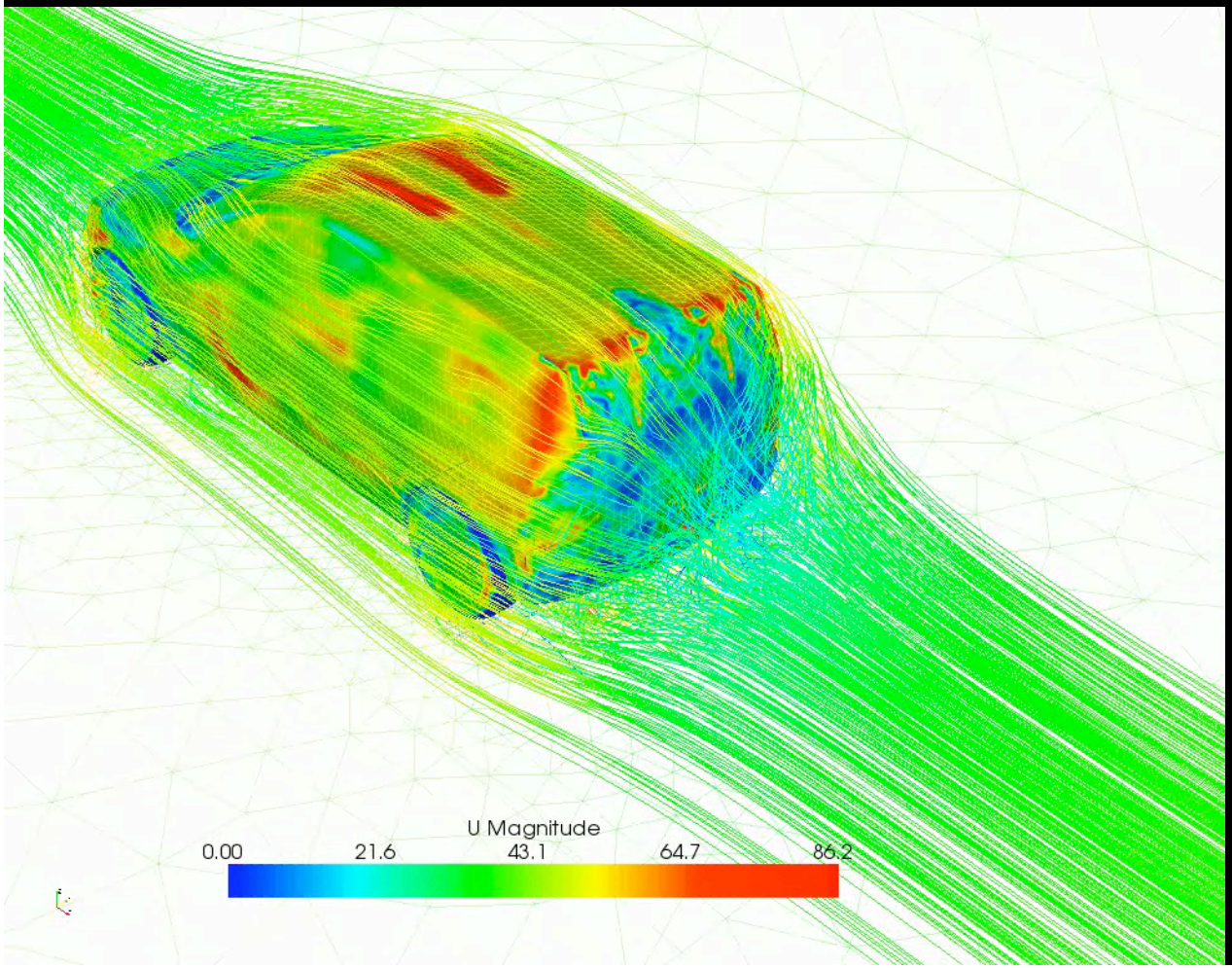
- Simulera verkligheten (lös ekvationen): numerisk metod + dator

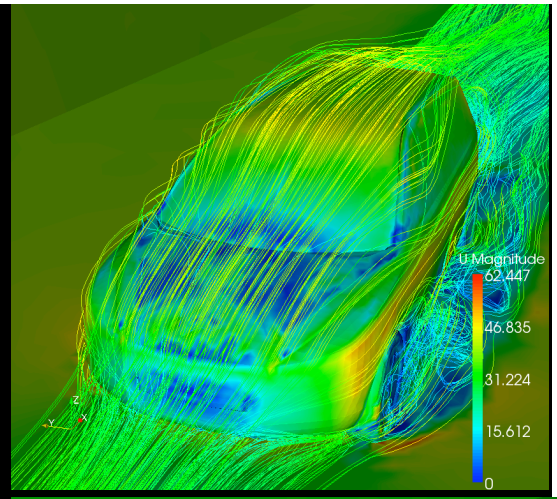
Tacoma Bridge 1940

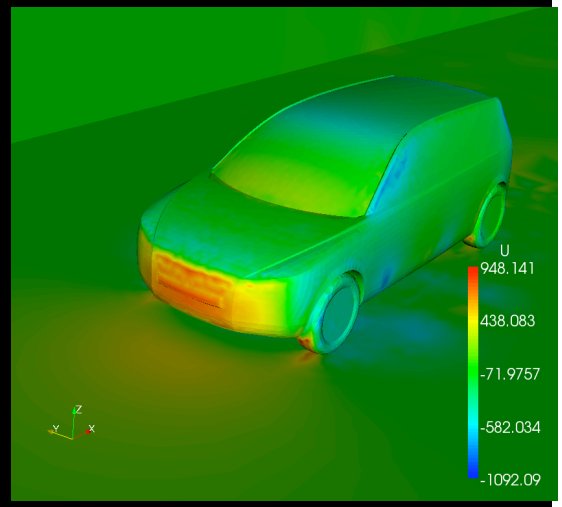


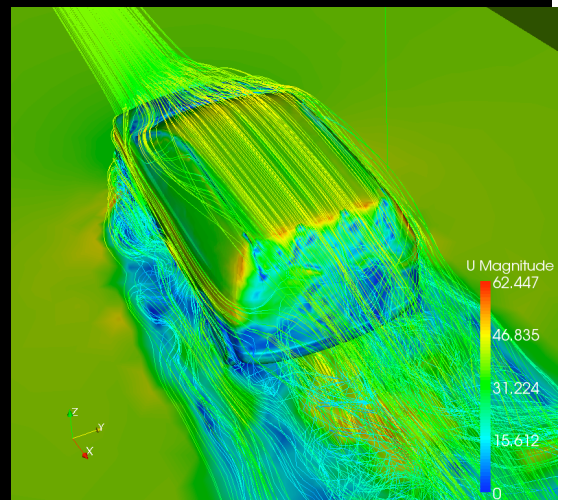
Modell: vind som blåser kring en elastisk struktur

Prototyp av Volvo [NA projekt]



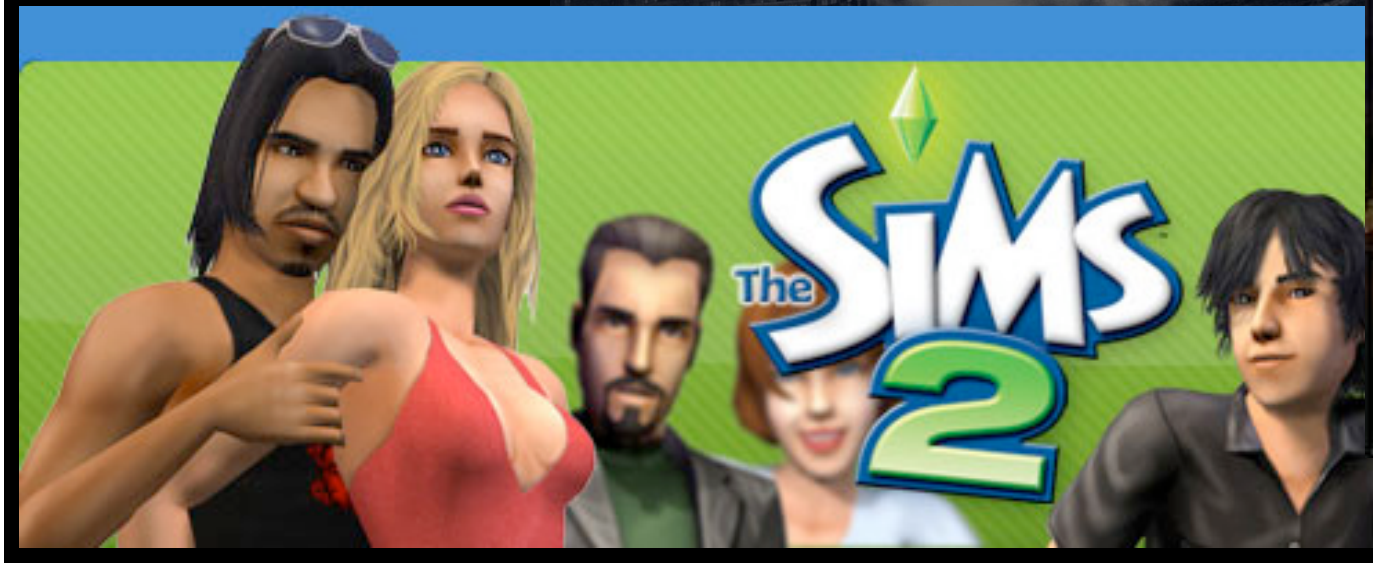




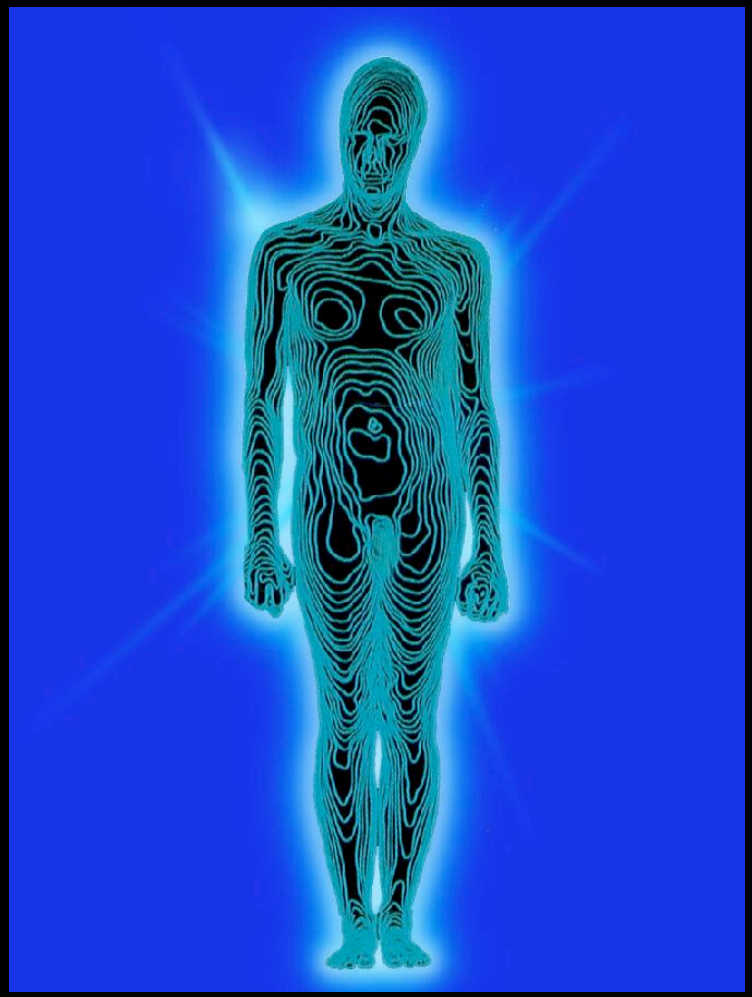


Dataspel & Film

- Upplevelsen ofta viktigare än realismen
- Fysikmotor
- Beräkningsfel ok

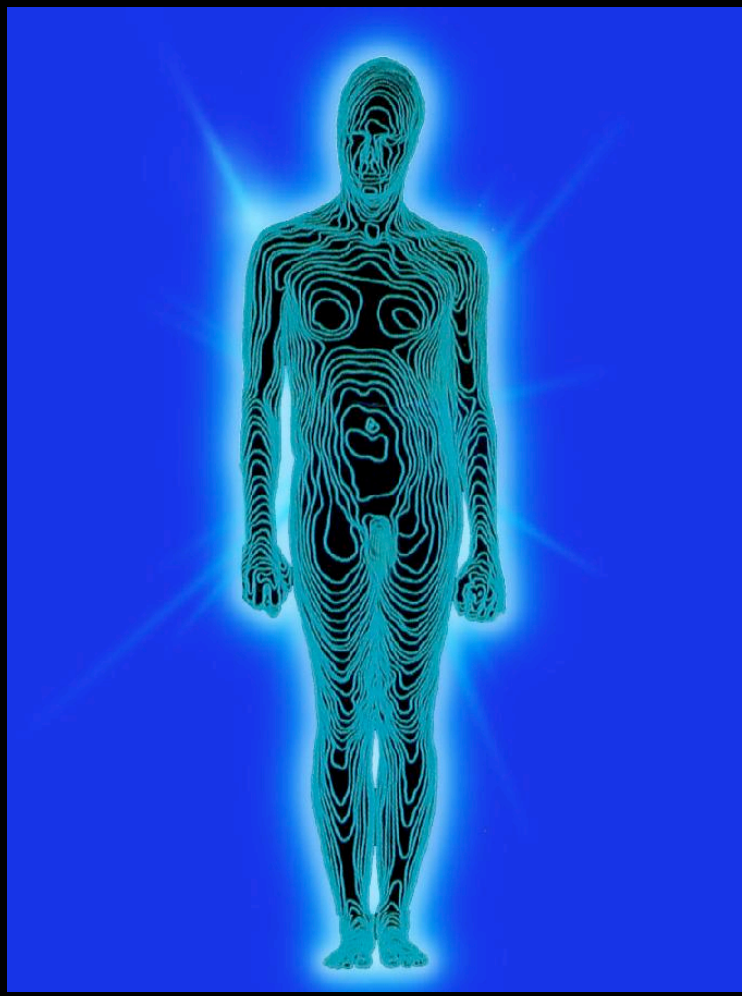


eHealth

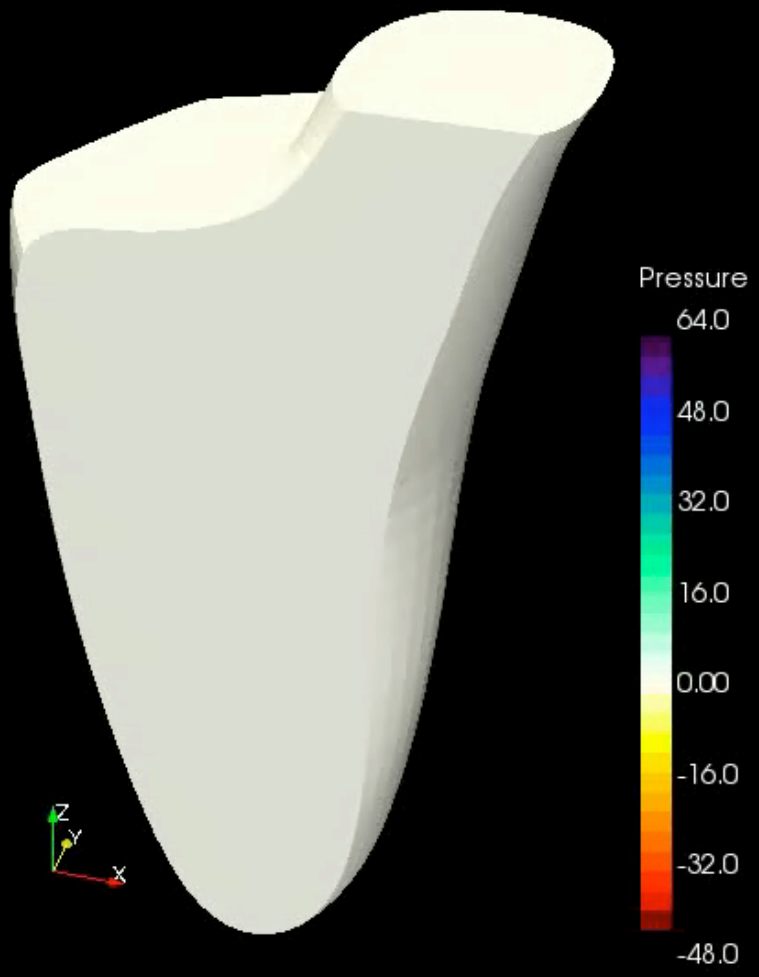


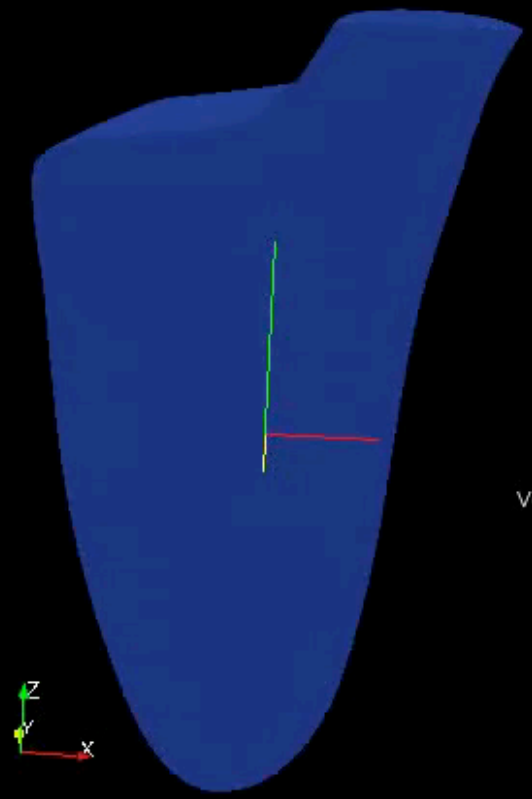
Virtual Physiological Human

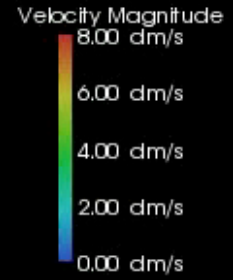
Deciding what treatment to give patients with serious illnesses, organ failure or even genetic disorders can present doctors with great difficulties. Whilst their potential benefits are clear, complex treatments often have both predictable and unpredictable side effects, and so there are always risks attached to any given choice. Information and Communication Technologies (ICT) can provide medical professionals with tools to model and predict the effects of different treatment options in individual patients.



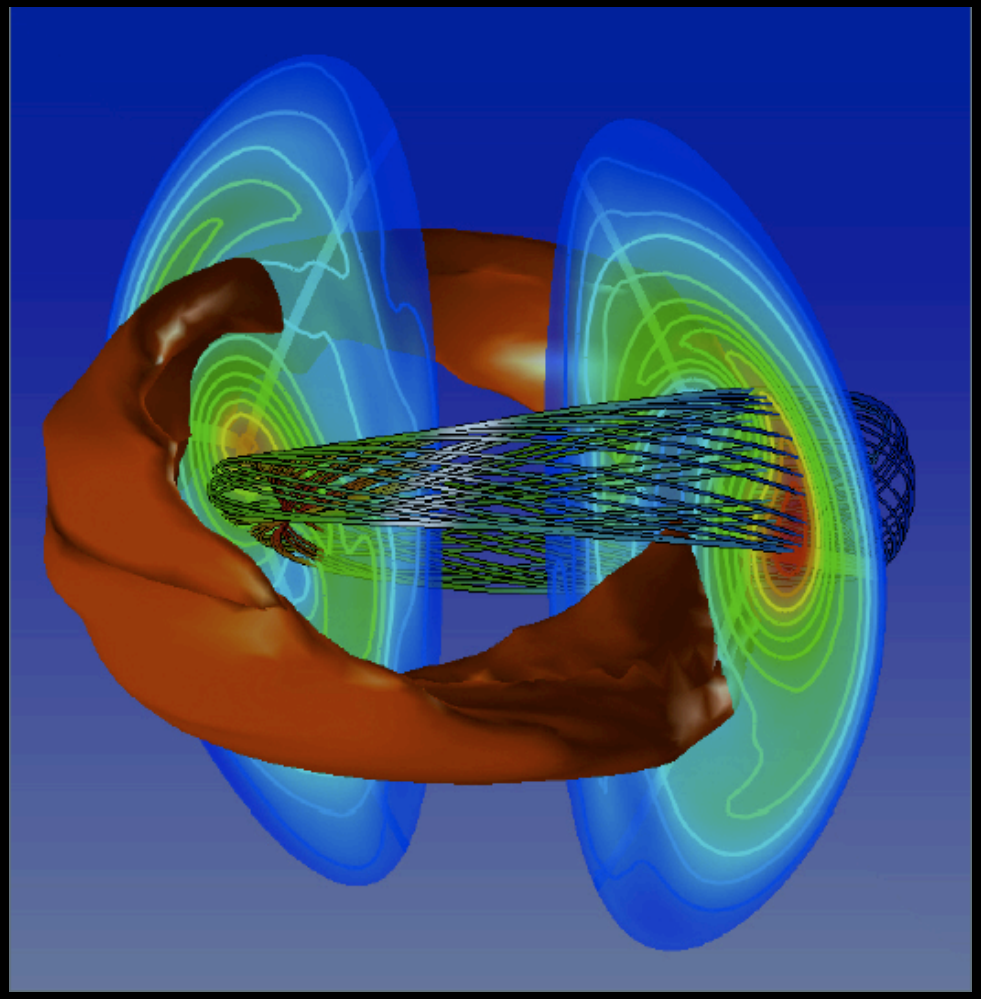
Virtuellt hjärta
[NA projekt]





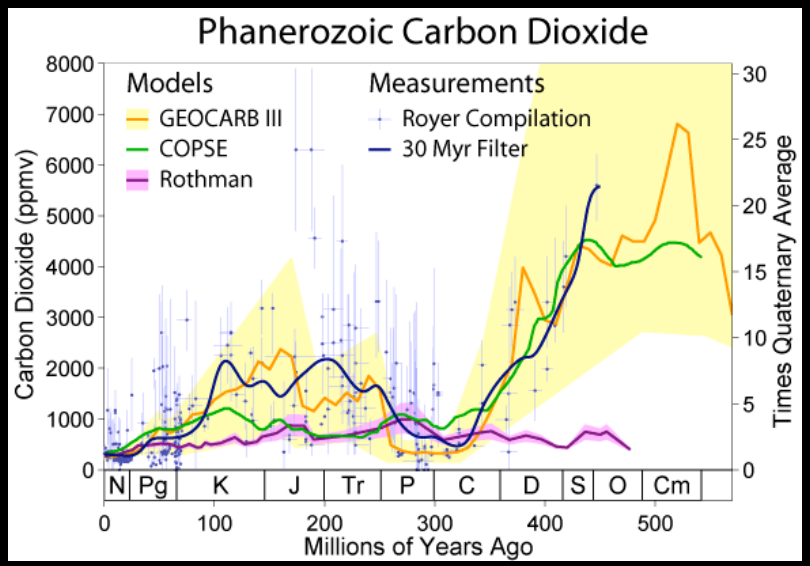


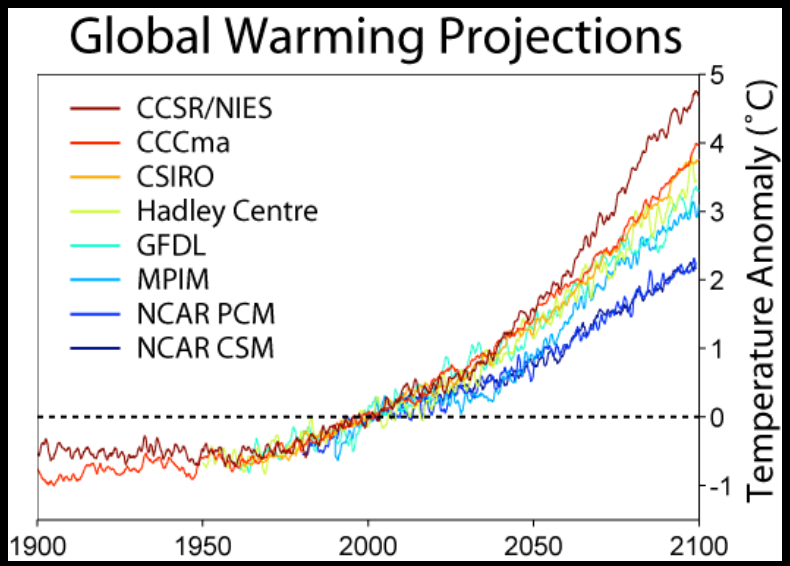
ITER: Fusion 2019?



Klimatmodeller

- Politiska beslut baseras på simulering
- Vilken modell?
- Noggrannhet?

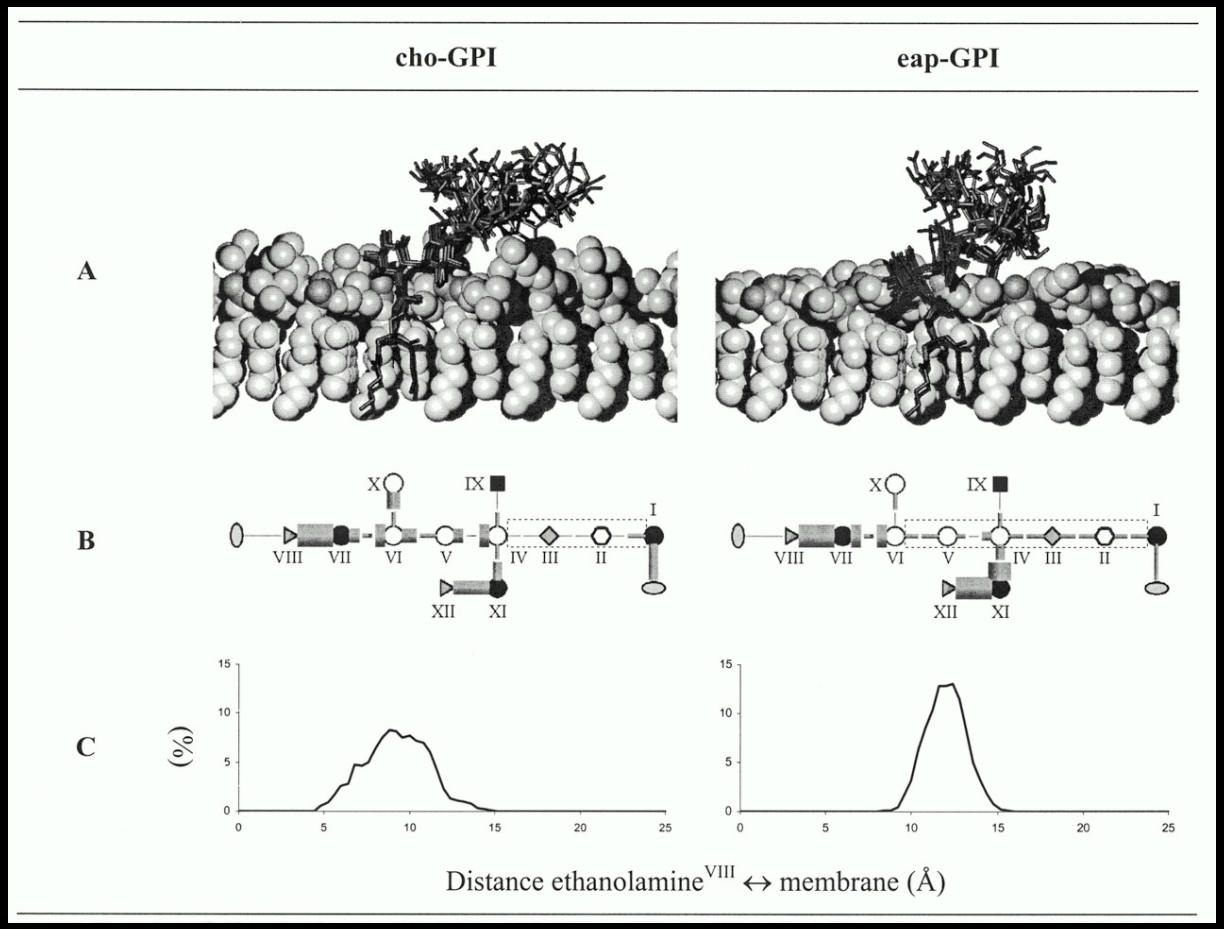




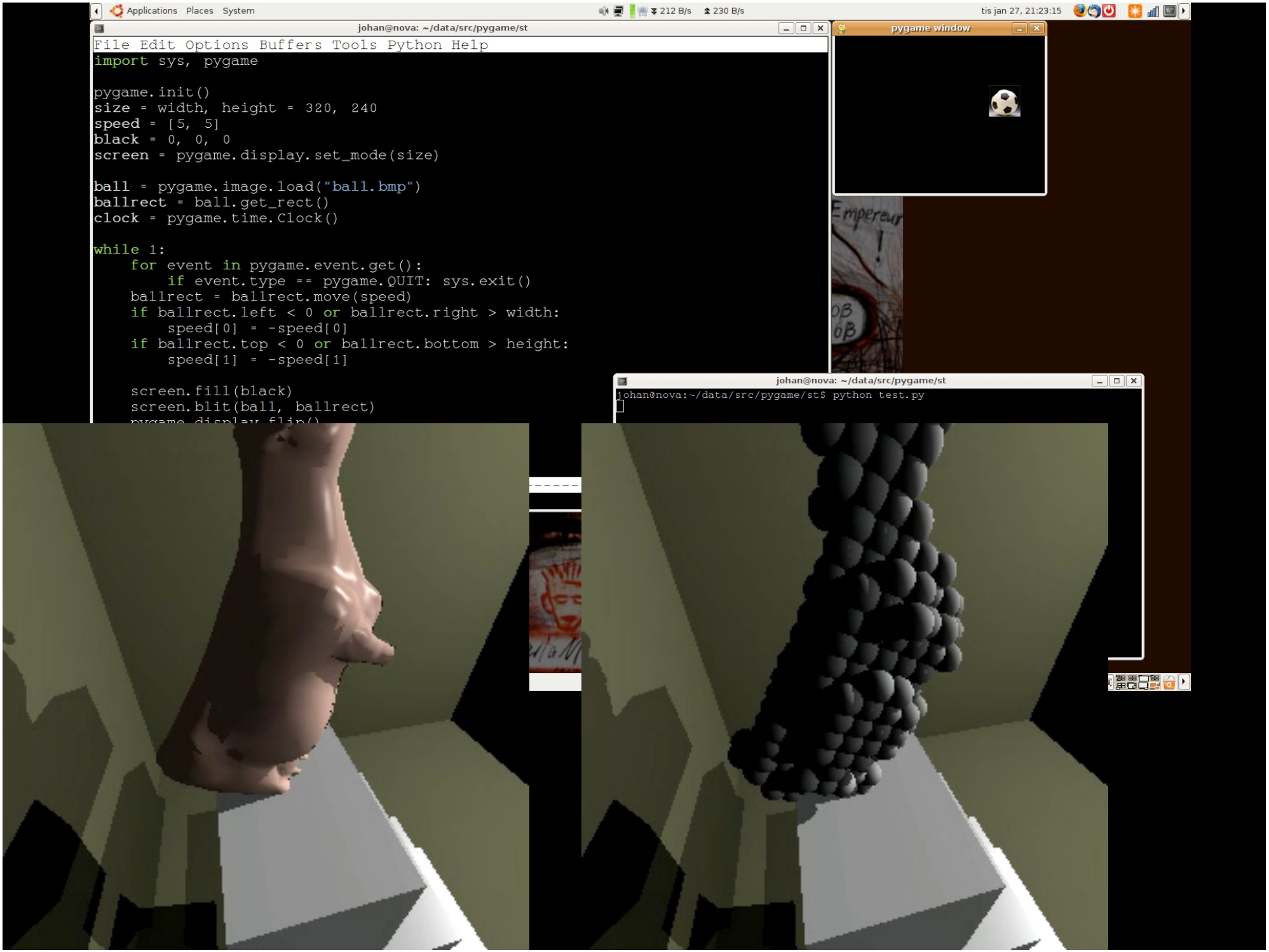
Denna kurs

- Matematiska modeller
- Numeriska metoder
- Implementering
- Simulering
- Uppskatta fel i simuleringen

Molekyldynamik - partikelmodell

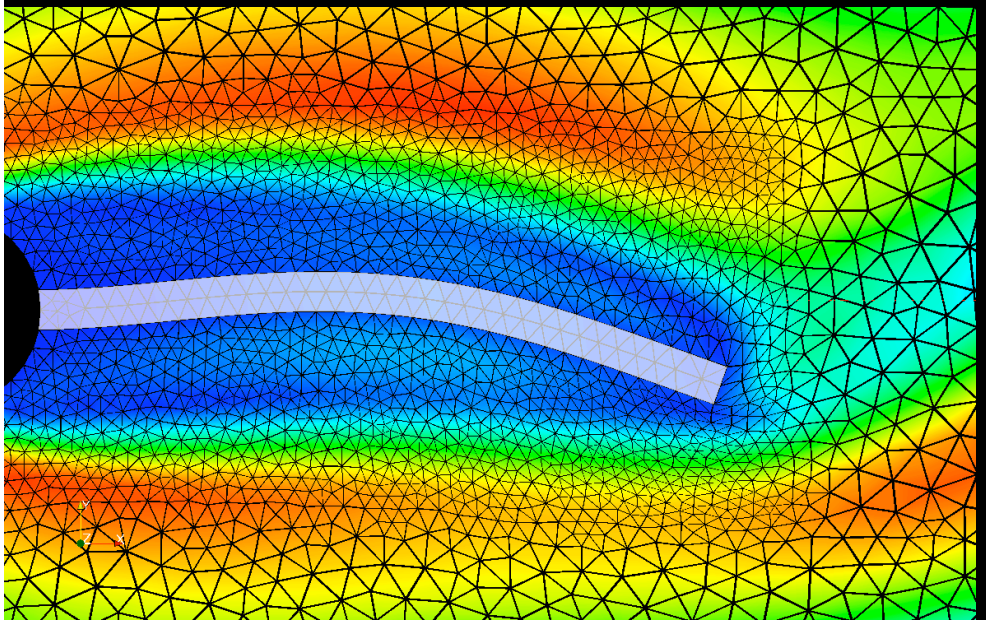


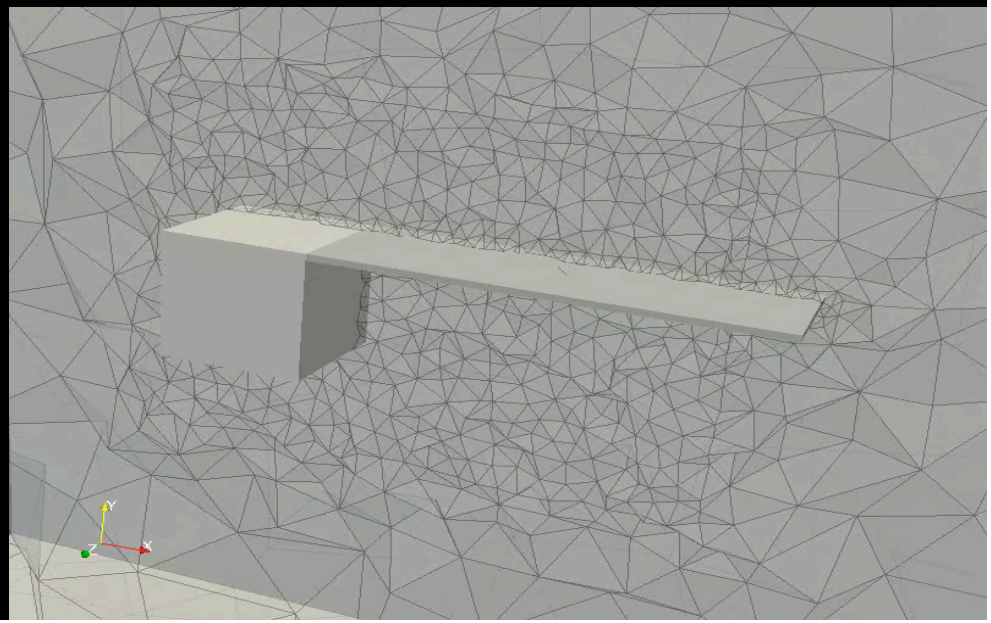
Virtual drug design


Applications Places System
212 B/s 230 B/s
tis jan 27, 21:23:15
johan@nova: ~/data/src/pygame/st
File Edit Options Buffers Tools Python Help
import sys, pygame
pygame.init()
size = width, height = 320, 240
speed = [5, 5]
black = 0, 0, 0
screen = pygame.display.set_mode(size)
ball = pygame.image.load("ball.bmp")
ballrect = ball.get_rect()
clock = pygame.time.Clock()
while 1:
for event in pygame.event.get():
if event.type == pygame.QUIT: sys.exit()
ballrect = ballrect.move(speed)
if ballrect.left < 0 or ballrect.right > width:
speed[0] = -speed[0]
if ballrect.top < 0 or ballrect.bottom > height:
speed[1] = -speed[1]
screen.fill(black)
screen.blit(ball, ballrect)
pygame window
johan@nova: ~/data/src/pygame/st
johan@nova:~/data/src/pygame/st$ python test.py

Differentialekvationer

- Beskriver kontinuum/fält/funktioner: temperatur, hastighet, tryck, densitet, etc.
- Finita element metoden: approximera lösningen med enkla funktioner på en triangulering





Eulers ekvationer (1755)

$\partial u/\partial t + u \cdot \nabla u + \nabla p = f$ Strömningsmekanik

$\nabla \cdot u = 0$

Maxwells ekvationer (1873)

$\partial B/\partial t + \nabla \times E = 0$

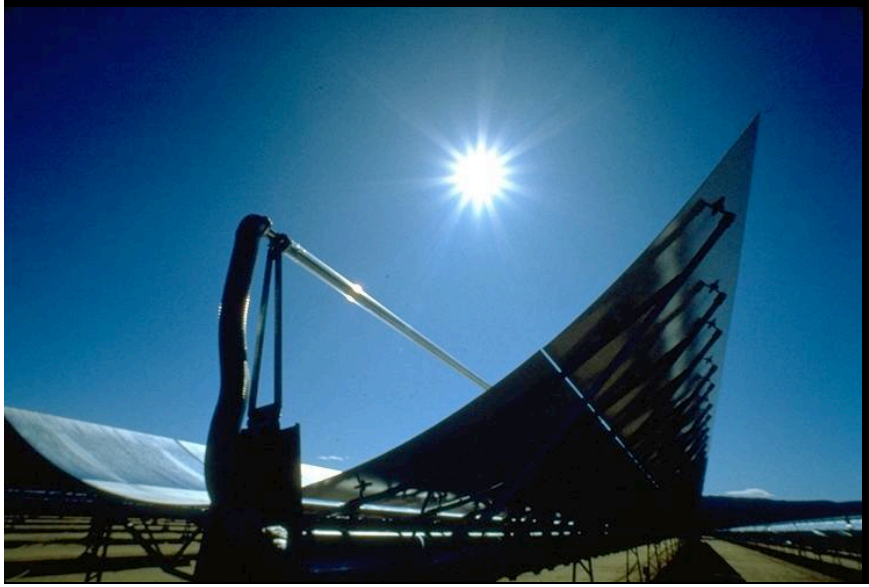
$\partial D/\partial t + \nabla \times H = 0$

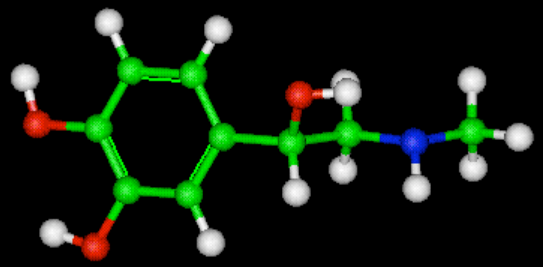
$\nabla \cdot D = 0,\ \nabla \cdot B = 0$

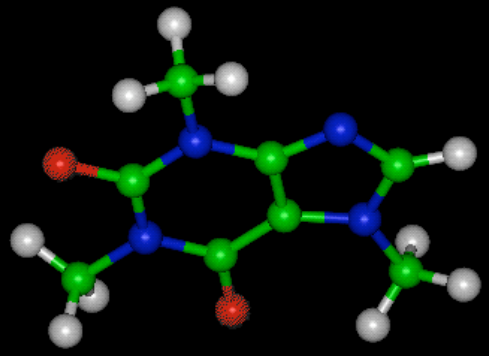
Elektromagnetism

Schrödingers ekvation (1925)

$i\partial\psi/\partial t = H\psi$ Kvantmekanik







Simulering ofta nödvändigt

- För små skalor för experiment
- För stora skalor för experiment
- Experiment oetiska
- Experiment dyra
- Simulera framtiden
- Simulera virtuell verklighet
- …

5-dygnsprognos

- Samla in data från väderstationer
- Simulera vädret med Eulers ekvationer

Varför inte 10-dygnsprognos?

- Samla in data från väderstationer
- Simulera vädret med Eulers ekvationer