Introduction

Modelling and Simulation, M.Biehl

Partly inspired by M. Wilkinson's introduction to the course Thanks to N. Caticha, Univ. Sao Paulo, for drawing my attention to Picasso's Bull

General Information

The course will give an introduction to

- some concepts and techniques of modelling and (computer) simulation
- in terms of examples from chaos theory, physics, biology, computer science
- with emphasis on
 - mathematical approaches
 - computational tools
 - numerical methods

Nestor page:

- announcements and news
- course documents (slides, additional material...)
- assignments
- secondary literature

Preliminary (!) list of topics

I Non-linear maps and chaotic dyn.

- -I.1. The logistic map
- I.2. Random number generators
- -I.3. Chaotic pendulum

II Aggregation and growth processes

- -II.1. Random walks
- -II.2. Fractal aggregates
- -II.3. t.b.a.

III Neural Networks

- -III.1. Biologically inspired models
- -III.2. Associative memories

Alternatives:

- Stochastic optimization
- Ising model of magnetism

Model formulation / methods

- -discrete iteration, visualization
- -dto.
- -ordinary diff. eqs. / num. integration

- -time/space discrete, random process
- –dto. + continuum, ordinary diff. eqs.
- Monte Carlo simulation

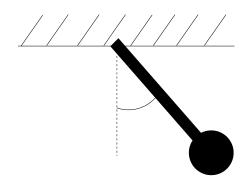
- -differential eqs., num. integration
- -discete system, Monte Carlo type sim.

Modelling

- (Mathematical) Modelling is required in almost all scientifi disciplines
- ... reduces potentially complex systems to its most essential features
- ... allows to treat the system mathematically and understand its properties
- ... requires a certain level of abstraction and simplificatio

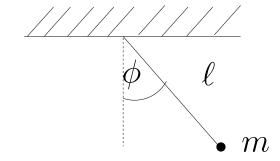
A simple example:

physical pendulum:



- ... consists of, e.g. a massive rod and a ball
- is subject to friction (suspension, air)
- kinetic energy depends on the actual shape
- potential energy depends non-linearly on ϕ

mathematical pendulum:



- ... a massless string and a point-like mass
- no friction (initial energy conserved forever)
- its kinetic energy is $1/2 \, m \, \ell^2 \, \dot{\phi}^2$
- its potential energy is $V(\phi)=mg\ell(1-cos[\phi])$ which **only for small** ϕ is *harmonic:* $V(\phi)\propto\phi^2$
- ... then, can be solved analytically
- ... helps to understand the real world pendulum
- -... doesn't exist

The quality of a model may be judged according to

- the model complexity, e.g.
 the number and nature of assumptions made
 the number of (free) parameters
 Occam's razor: if different ideas can explain the same thing, accept the simplest
- the possibility to simulate or even solve the model analytically
- the faithful representation of system details
- the range of applicability
 the latter two aims usually conflict

• its universality:

the (mathematical) structure of very different systems can be surprisingly similar: fractal aggregates: crystal surfaces, ..., bacteria colonies synchronization of: coupled pendula, ..., neural networks dynamics of : disordered magnets, ..., stochastic optimization

• its predictive power

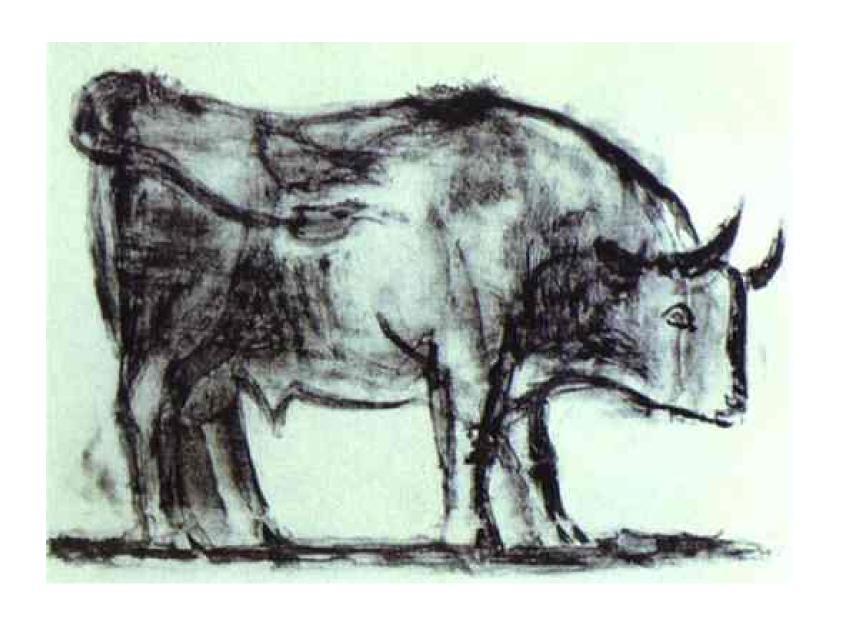
- accuracy of qualitative/quantitative predictions
- can we only reproduce and understand known properties or can we predict novel features of the system?

The appropriate level of simplification/abst action depends on

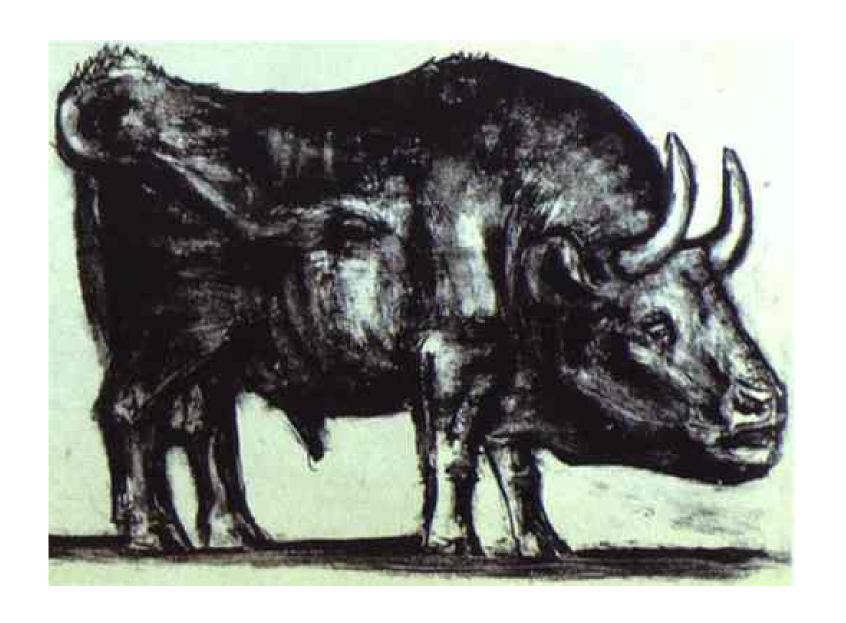
- the aim of modelling, e.g.
 predicting the weather for a few days vs.
 modelling the long term evolution of the world climate
- the available analytical tools or computational power we may be able to model a single neuron (atom) in great detail but how about 10^{12} neurons in the brain (10^{23} atoms in a crystal)?

The art of modelling boils down to

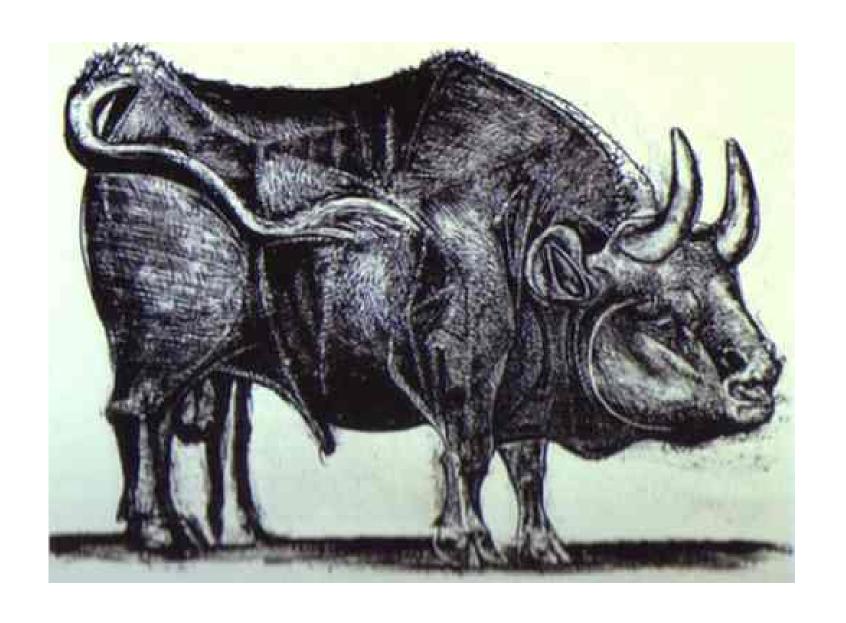
- leaving out details that are irrelevant for the investigated problem
- keeping the necessary features which allow to understand the system and make predictions



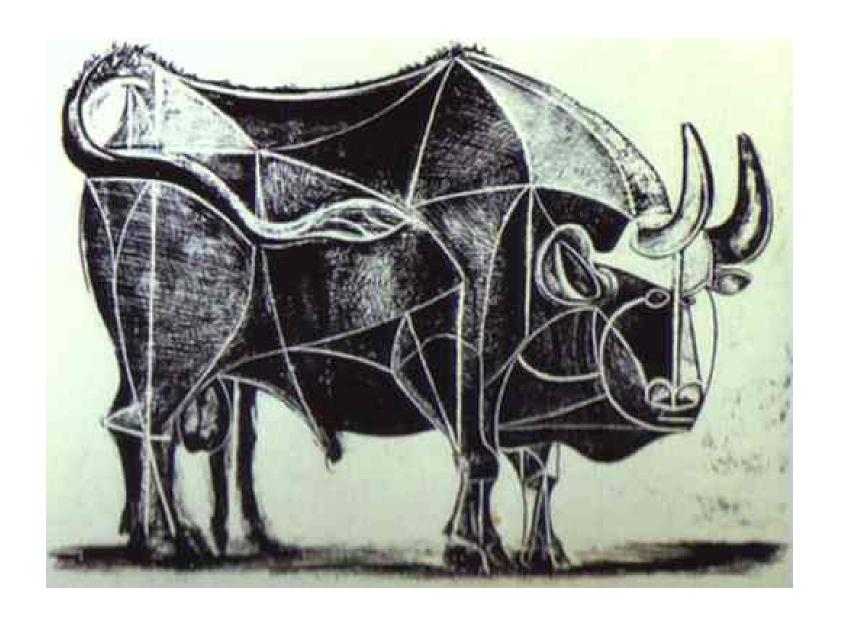
Pablo Picasso, The Bull I, 1945



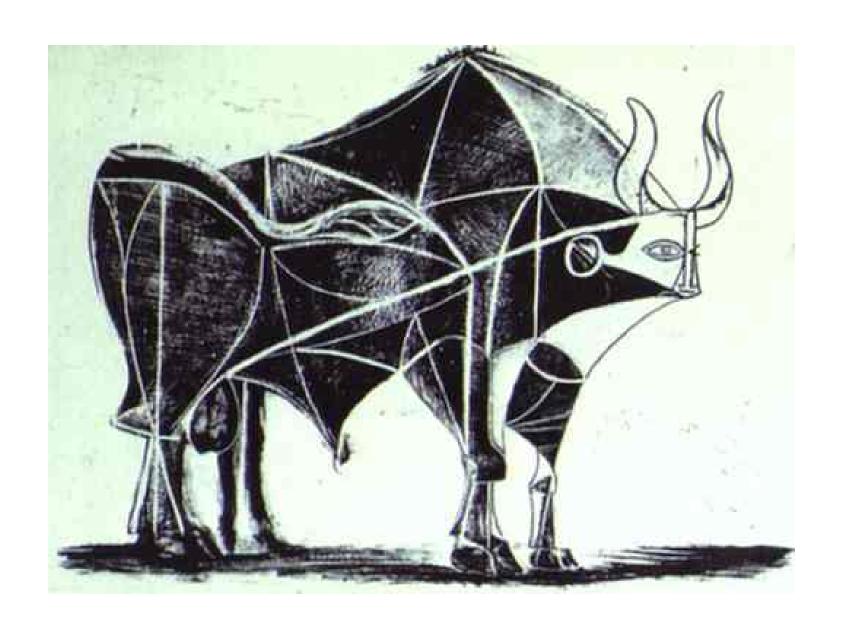
Pablo Picasso, The Bull II, 1945



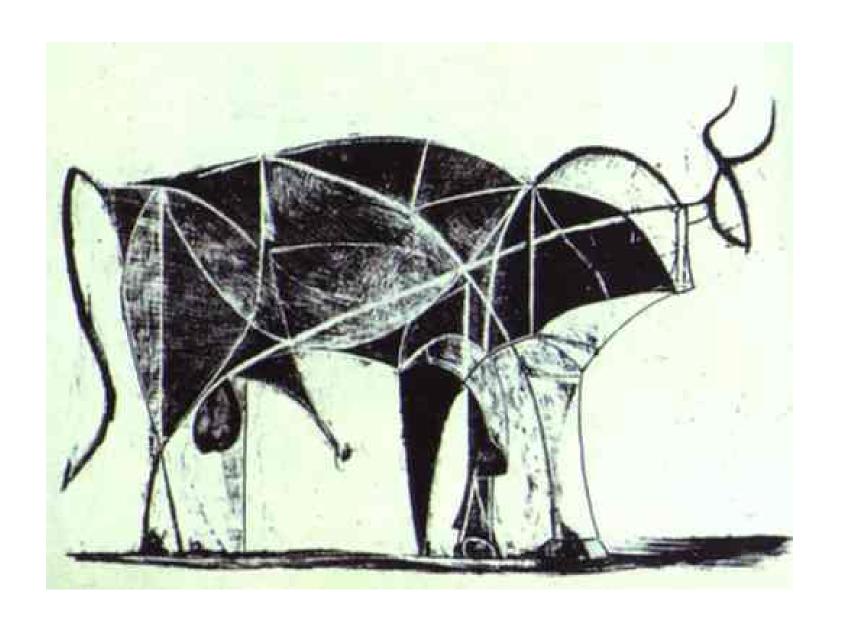
Pablo Picasso, The Bull III, 1945



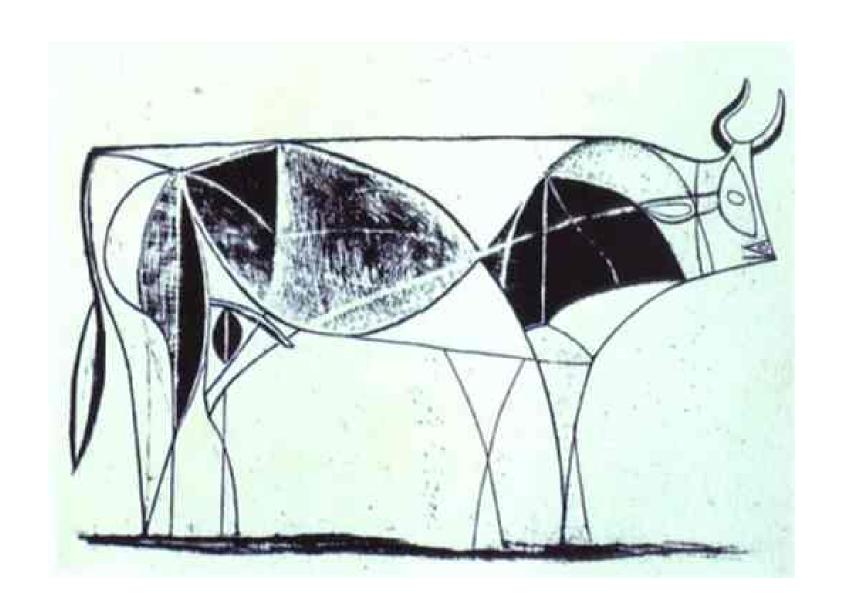
Pablo Picasso, The Bull IV, 1945



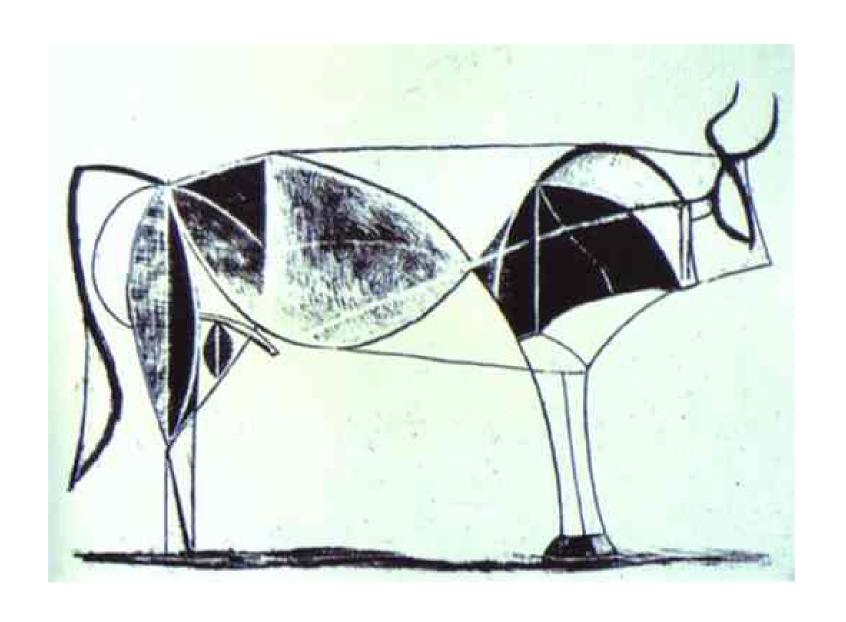
Pablo Picasso, The Bull V, 1945



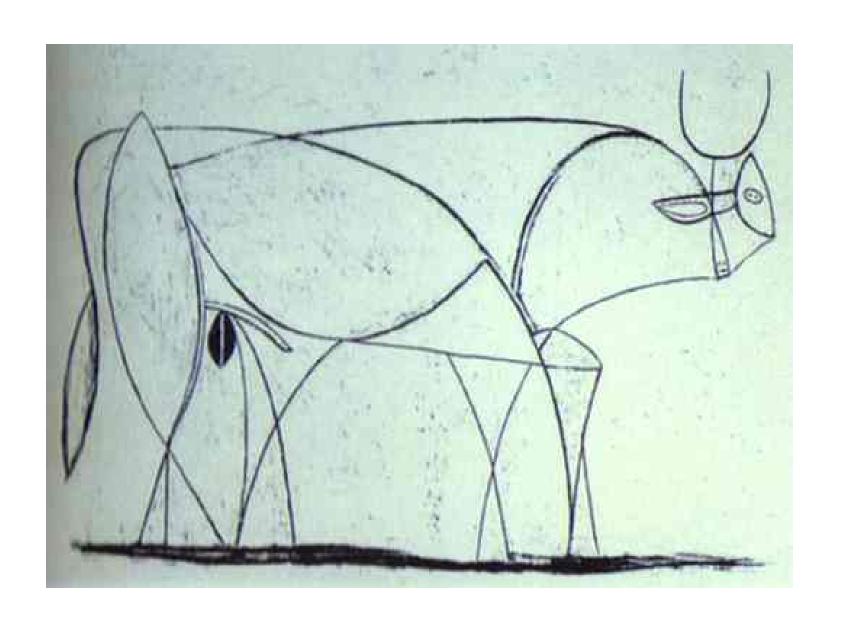
Pablo Picasso, The Bull VI, 1945



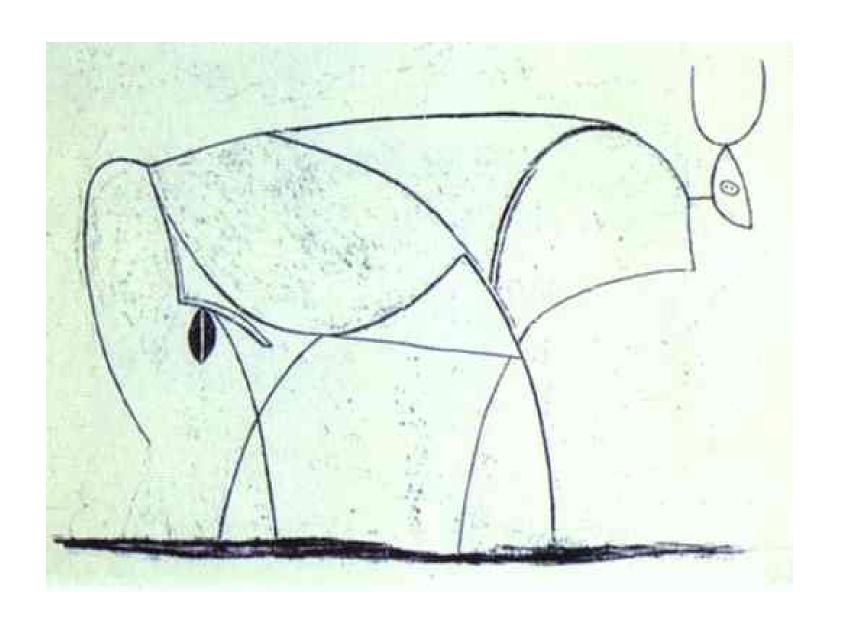
Pablo Picasso, The Bull VII, 1945



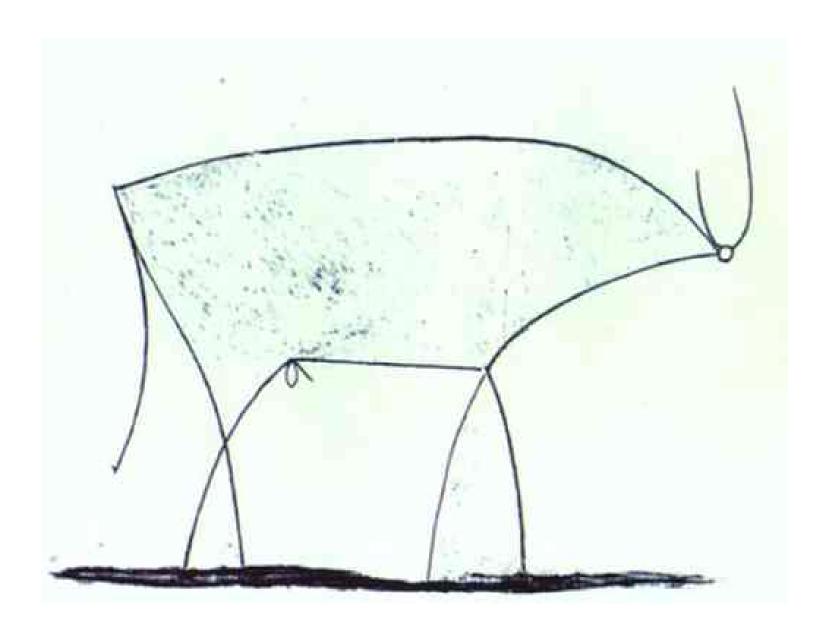
Pablo Picasso, The Bull VIII, 1946



Pablo Picasso, The Bull IX, 1946

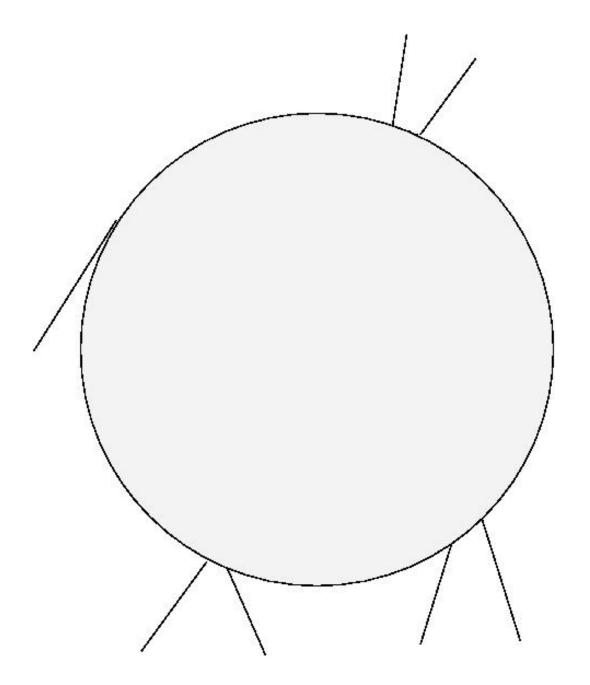


Pablo Picasso, The Bull X, 1946



Pablo Picasso, The Bull XI, 1946

A. Einstein: A model should be as simple as possible ...



Michael Biehl, The Cow, 2004

... but no simpler