
# Introduction to Scientific Computing

(Lecture 1)

Bojana Rosić

Institute of Scientific Computing

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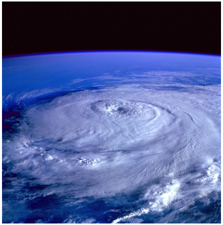
# Why scientific computing?

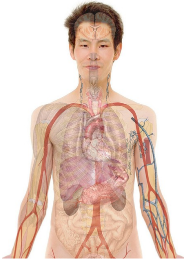
*Prediction obtained by computer simulation sometimes can be the only information one may have.*

New Horizons

# Modelling and prediction

*Almost everything around us can be described by a* **mathematical model***, and hence* **simulated on computer***. The modelling of for example human body, climate change, floods etc. can help us to prevent disasters. Also, numerical simulations can help us to reduce cost of production or to improve the existing environmental state.*

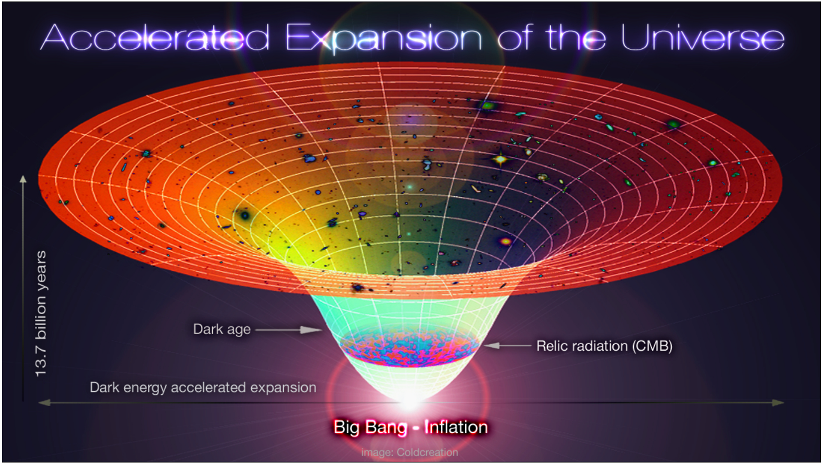




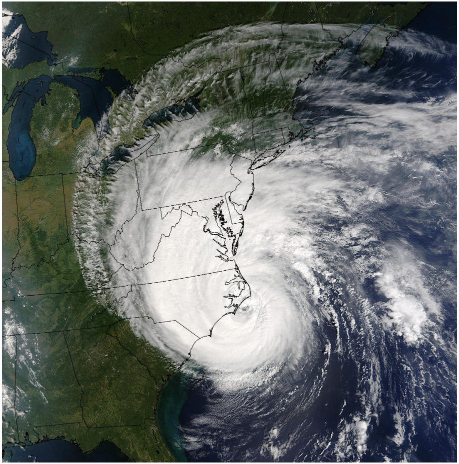
# Time

*"What was there before the big bang? Well, you see, there was no before because before the big bang, time did not exist.* **Time is a result of the expansion of the universe itself**. *But what will happen when the universe has finished expanding?"- Adult Nemo, Mr Nobody, Jaco Van Dormael, 2009*

# Our topic: time dependent systems



# Our topic: time dependent systems



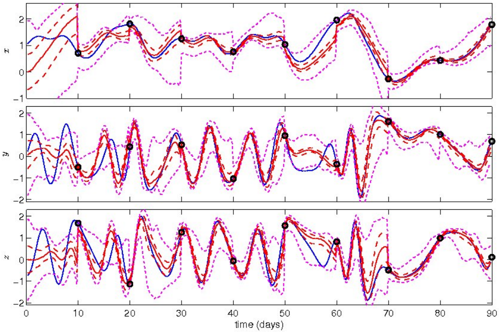
camp.cos.gmu.edu

# Our topic: time dependent systems

cyclix.com

# Time dependent system = dynamical system

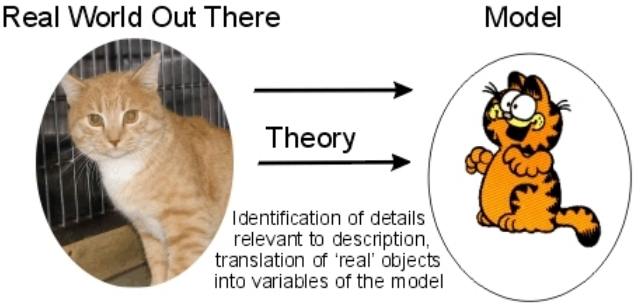
System that evolves over time possibly under external excitations. The dynamics of the system is the way the system evolves and the dynamical model is a set of mathematical laws that describe the system up to certain precision.



# Goals

- model the time dependent phenomena (dynamical system), i.e. map the real world to the mathematical model. This is part of other subjects such as mechanics, thermodynamics, etc.
- given the model, simulate and predict its response. The model and real system response have to match. **This is our goal**.
- make decisions by having the system response, i.e. control the system, improve it, etc. This is part of other subjects: system control, robotics, etc.

# Real world to mathematical model




*http://www.prime-spot.de/Bilder/BR/theoryandmodel.jpg*

# Real world to mathematical model

Dynamical system is described by:

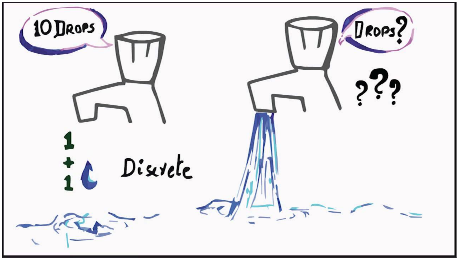
- **time**
- **the state** $x$ — a collection of coordinates that describe all the modeler feels is needed to give a complete description of the system.
- **the evolution rule** — provides a prediction of the next state or states that follow from the current state space value.

Poincare (@wiki)

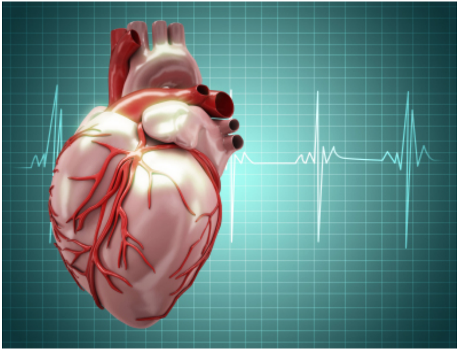
# Real world to mathematical model

With respect to time, the dynamical system can be

- **discrete** — system in time is described by a finite number of states $x(t_i), i = 1, ..., N$
- **continuous** — system in time is described by infinite number of states $x(t)$



# Real world to mathematical model



continuous

.escardio.org

discrete

sheknows.com

# Continuous model: differential equations

*A differential equation is a mathematical equation that relates some function of one or more variables with its derivatives*

- **Ordinary differential equation (ODE)**: single independent variable

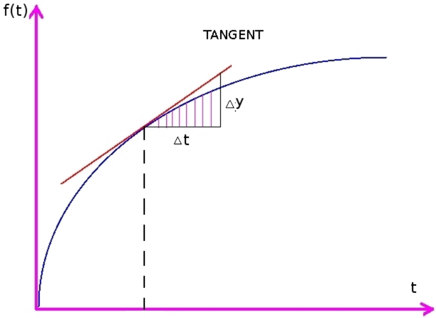
$$\frac{du}{dt} = 5t + u^2 \quad \text{time dependent}$$

- **Partial differential equation (PDE)**: several independent variables

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 2x^2 \quad \text{time independent}$$

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial u}{\partial t} = 5(x+y) \quad \text{time dependent}$$

# Meaning of time derivative in ODE

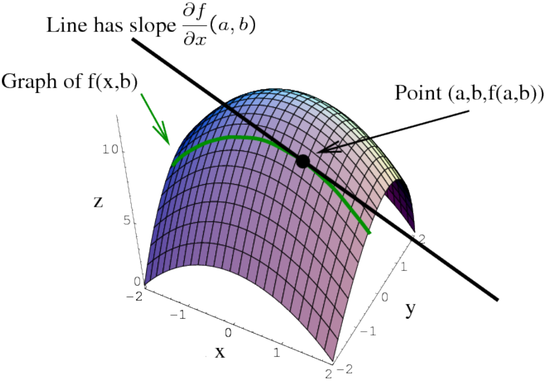



*Time derivative represents* **the change of quantity** $y = f(t)$ *in infinitesimal interval of time.*

$$f'(t) = \frac{df}{dt} = \lim_{\Delta t \to 0} \frac{\Delta y}{\Delta t}$$

# Meaning of partial derivatives in PDEs

$$z = f(x, y)$$




*mathinsight.org*

# Discrete model: difference equations

*A difference equation is a mathematical equation that relates two or more elements of a sequence.*

$$\Delta x_{n+1} = 3x_{n+1} - x_{n+2}$$

i.e.

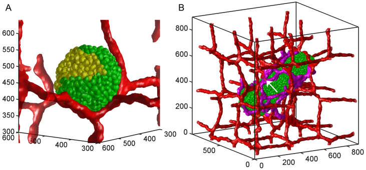
$$x_{n+1} - x_n = 3x_{n+1} - x_{n+2}$$

Here, $x_n$ is the $n - th$ element of a sequence.

## Continuous: Tumor growth

**State:** number of tumor cells $N$ From **medical experience** one may model the tumor growth as:

$$\frac{dN}{dt} = \left(\frac{\mu N}{\nu}\right)\left[1 - \left(\frac{N}{K}\right)^{\nu}\right], \quad \mu > 0$$




doi:10.1371/journal.pone.0007190

in which $\mu$ and $\nu$ are the model parameters. The treatment by a chemical agent with strength $\alpha$ and concentration $c(t)$ changes the previous equation to

$$\frac{dN}{dt} = -\alpha c(t) N + \left(\frac{\mu N}{\nu}\right)\left[1 - \left(\frac{N}{K}\right)^{\nu}\right]$$

Source: Sachs et al., Simple ODE models of tumor growth and anti-angiogenic or radiation treatment, *Mathematical and Computer Modelling*, Volume 33, Issues 12–13, June 2001, Pages 1297–1305

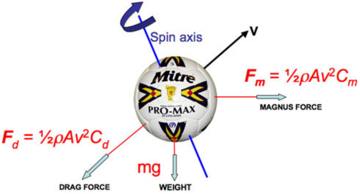
# Continuous: Spinning ball

**State:** the position of ball $(x, y, z)$. From **aerodynamics** one may model the spinning as:

$$\frac{d^2x}{dt^2} = -vk(C_d\frac{dx}{dt} + C_m\frac{dy}{dt})$$

$$\frac{d^2y}{dt^2} = -vk(C_d\frac{dy}{dt} - C_m\frac{dx}{dt})$$

$$\frac{d^2z}{dt^2} = -g - vkC_d\frac{dz}{dt}$$



www.math.org

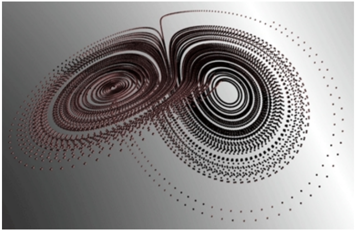
Here, $v$ is the total speed, $k = \frac{\rho A}{2m}$, $m$ is the mass of the ball, $C_d$ is the drag coefficient and $C_m$ is the Magnus force coefficient.

Source: Bray et al., Modelling the flight of a soccer ball in a direct free kick, *J. of Sports Sciences*, Vol 21, pp 75-85, 2003.

# Continuous: atmospheric Lorenz convection

**State:** $(x, y, z)$ ($x$ represents a symmetric, globally averaged westerly wind current, whereas $y$ and $z$ represent the cosine and sine phases of a chain of superposed large-scale eddies transporting heat polewards.)

$$\frac{dx}{dt} = a(y - x)$$
$$\frac{dy}{dt} = x(b - z) - y$$
$$\frac{dz}{dt} = xy - cz$$



copyright by Ian Stewart

They also represent simplified models for lasers, dynamos, thermosyphons, brushless DC motors, electric circuits, chemical reactions and chaos in brain.

## Continuous: Schrödinger equation

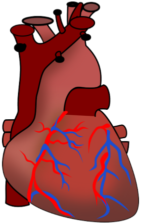
The analogue of Newton's law is Schrödinger's equation for a quantum system describing the time-evolution of the system's wave function (also called a "state function")

$$i\hbar \frac{\partial}{\partial t}\Psi = \hat{H}\Psi.$$

copyright by The Big Bang Theory

where $i$ is the imaginary unit, $\hbar$ is the Planck constant divided by $2\pi$ (which is known as the reduced Planck constant), $\Psi$ is the wave function of the quantum system, and $\hat{H}$ is the Hamiltonian operator.

# Continuous: Heart beat



**State**

- length of muscle fiber $x$
- electrochemical activity $b$

From **interdisciplinary expertise** one may model the heart beat as:

$$\epsilon \frac{dx}{dt} = -(x^3 - Tx + b) \quad \text{and} \quad \frac{db}{dt} = (x - c) + U(x - d)$$

where $T$ is the overall-tension of the system, $U$ is the step function and $c$ and $d$ are constants describing diastole (relaxed state) and systole (contracted state).

# Discrete: Bank account

- balance of the bank–account after the $n$–th year: $x_n \in \mathbb{R}, (n \geq 0)$
- initial balance: $x_0 \in \mathbb{R}$
- rate of interest: $p$

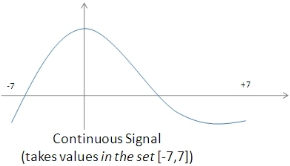
Moreover let

$$\Delta x_n := x_{n+1} - x_n$$


Then the resulting annual change is

$$\frac{\Delta x_n}{x_n} = p \quad \Leftrightarrow \quad \Delta x_n = p x_n$$

# But,

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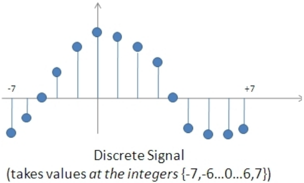



By **computer** simulation we transform

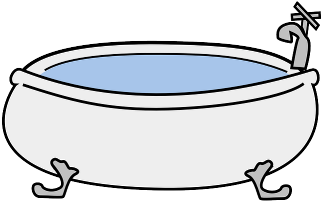
continuous to discrete system.

Our task is to do this transformation (called discretisation) in a best possible way without loosing any system property.

# Example: Bathtub

**State** is the water level given in

- inital time: $h_0$ (known)
- arbitrary time $t$: $h(t)$ (not known)



From **fluid mechanics** (*your expert knowledge*) we know that the speed of running water $\frac{dV(t)}{dt} = \frac{dAh(t)}{dt}$ is proportional to the depth of bathtub $h(t)$:

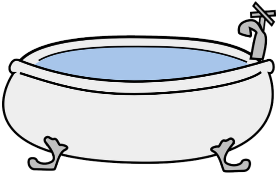
$$\frac{dV(t)}{dt} = A\frac{dh(t)}{dt} = -kh(t)$$

$$\Rightarrow \frac{dh(t)}{dt} = -\frac{k}{A}h(t) \quad \textbf{evolution law}$$

# Discretisation

The time derivative in the **differential** equation

$$dh/dt = -k/Sh$$



can be **approximated** by a finite difference, i.e.

$$\frac{dh}{dt} = \lim_{\Delta t \to 0} \frac{\Delta h}{\Delta t} \approx \frac{h(t_{n+1}) - h(t_n)}{\Delta t}$$

such that one obtains the **difference** equation:

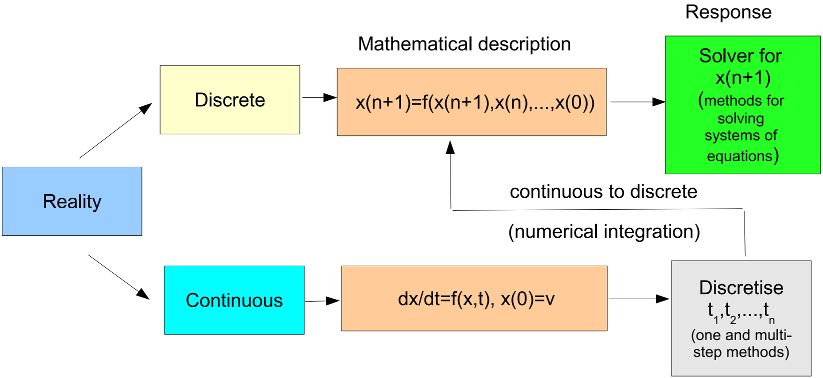
$$\frac{h_{n+1} - h_n}{\Delta t} = -\frac{k}{S} h_n \Rightarrow h_{n+1} = h_n - \frac{k}{S} h_n \Delta t$$

where $h_{n+1} = h(t_{n+1})$ etc.

# Is this the only way to do discretisation?

The transformation introduced previously is **NOT the only way**. There are **many other** schemes which can be used to transform the differential to difference equation. They are all characterised by different complexities and accuracies. Hence, in the next one year (ODE I and ODE II) we will study them.

# Program of this course



# Program of this course

- Simulation on computer: computer arithmetic
- Discrete dynamical systems (difference equations)
  - first order difference equations
  - higher order difference equations
  - stability
- Numerical methods for solving equations
  - fixed point iterations
  - stationary iterative methods
  - Krylov subspace methods
  - Newton type of methods

# Program of this course

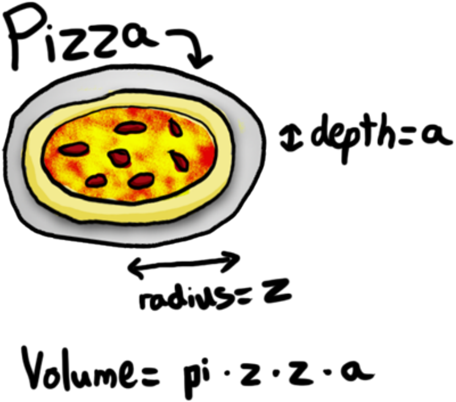
- Continuous dynamical systems (differential equations)
  - first order differential equations
  - higher order differential equations
  - stability
- Numerical integration (discretisation)
  - one-step methods
  - multi-step methods

# Literature

You may consider following sources:

- lecture and tutorial slides
- short lecture notes from our web-site
- E. Hairer and G. Wanner, Solving ordinary differential equations
- Michael T. Heath. Scientific computing: an introductory survey.
- Wei-Chau Xie, Differential Equations for Engineers
- after each lecture you will get new references

# After this course...




...**You should see the world in another perspective!**