Numerical Methods in Biomechanics

ME-484

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EPFL - Laboratory of Biomechanical Orthopedics

Content - schedule

W01: Organization, introduction and examples
W02: External lecturers
W03: Partial Differential Equations
W04: Solid mechanics in numerical biomechanics
W05: Fluid mechanics in numerical biomechanics
W06: The Finite Element Method (FEM), and its extensions
W07: Midterm project presentations
W08: Midterm evaluation
W09: Multiphysics and coupling
W10: Example 1
W11: Example 2
W12: Example 3
W13: Final project presentation

Partial Differential Equations

Most biomechanical systems can be described by

- A set of Partial Differential Equations (PDEs)
- Completed with constitutive equations
- Boundary conditions
- Initial conditions

PDEs

- Solid (deformation) mechanics (stress, strain)
- Fluid mechanics (fluid velocity, pressure)
- Heat (temperature)
- Transport (diffusion, advection, concentration)
- Electromagnetism (electric & magnetic potential)
- Wave propagations (EM, acoustic)
- Coupling in multi-physics

Ordinary Differential Equations (ODE)

- Differential equation of 1 dependent (function) variable y with 1 independent variable t
- Linear/nonlinear
- Order (highest derivative)
- Homogeneous/nonhomogeneous (source term)
- Existence, uniqueness (Cauchy–Lipschitz theorem)

$$\frac{dy}{dt} = F(t, y), y(t_0) = y_o$$

Ordinary Differential Equations (ODE)

- System of linear ODEs
- ODE of order n can reduce to n 1st order ODEs
- Non constant coefficients : $A = A(x, t)$
- Nonhomogeneous ODE ($b \neq 0$)
- Boundary problem (x), or initial value problem (t)

$$\frac{dy}{dt} = A \cdot y(t) + b(t), \qquad y(t_0) = y_0$$

ODE example: Lotka-Volterra

- Predator-prey model
  - Predators’ number rate depend on prey’s number
  - Prey’s number rate depend on predators’ number
  - With few predators, preys can reproduce
  - If predators over-exploit preys, they decrease
- Applied to animals, cells, chemicals
- Typically oscillating solutions

Jost et al., The wolves of Isle Royale display scale-invariant satiation and density dependent predation on moose, J. Anim. Ecol., 74(5), 809–816 (2005)

ODE example: Lotka-Volterra

P : predators (concentration)

H : prey (concentration)

r : growth rate of H

a : predation rate coefficient

b : growth rate of P

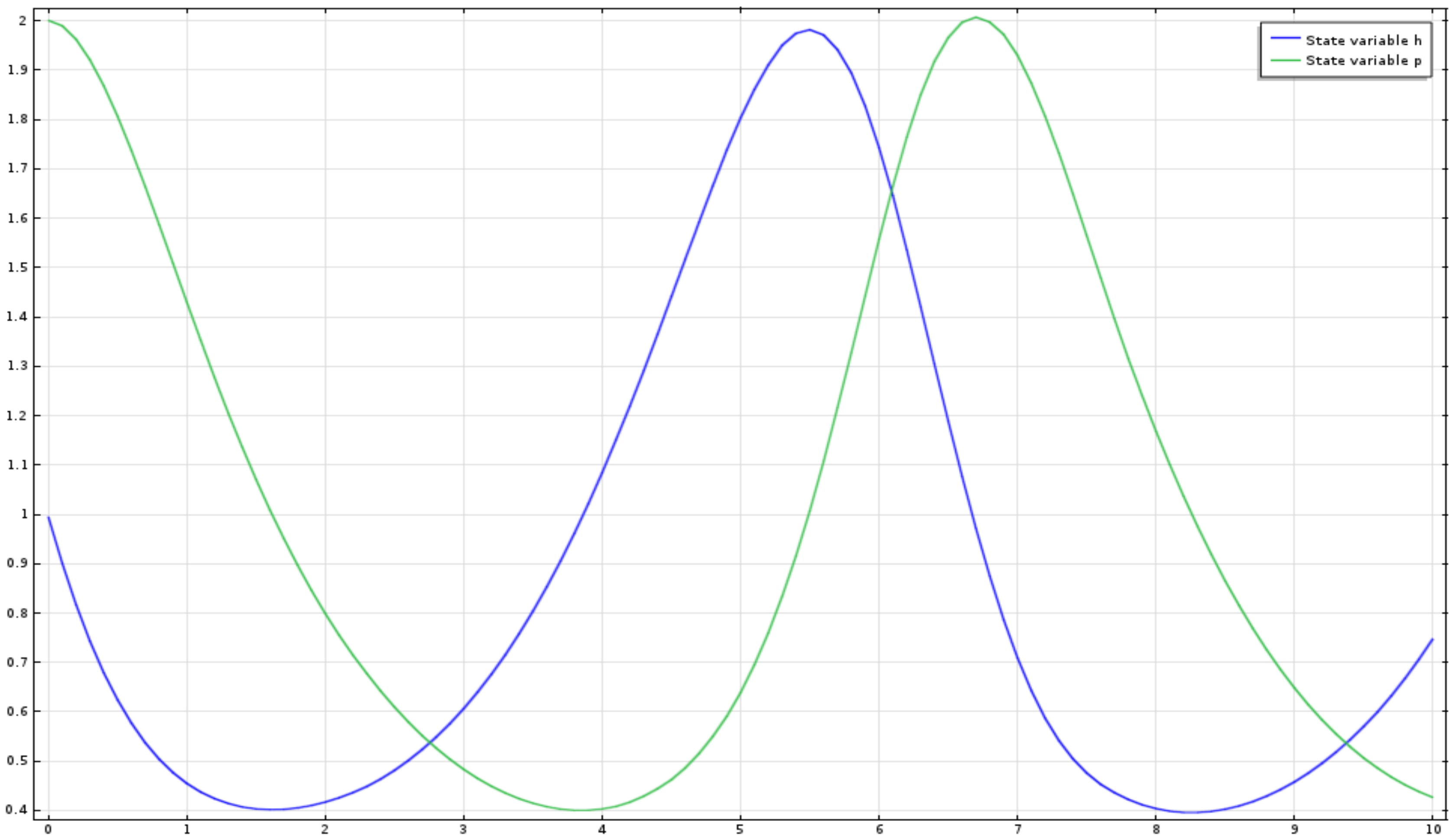
m : mortality rate of P

Constants: r = a = b = m = 1

Initial condition: $H(0) = 1$, $P(0) = 2$

$$\begin{cases} \dfrac{dH}{dt} = (r - aP)H \\ \dfrac{dP}{dt} = (bH - m)P \end{cases}$$

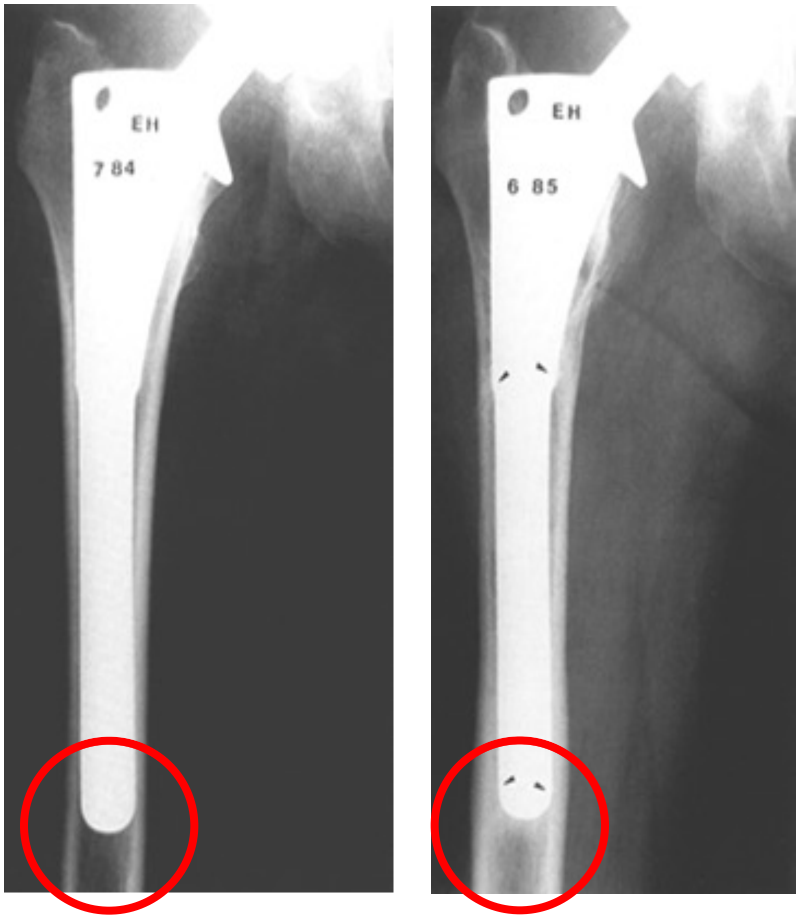
ODE example: Lotka-Volterra



Try with other initial conditions (stationary point: $H_0 = P_0 = 1$) or constants

ODE example: bone adaptation

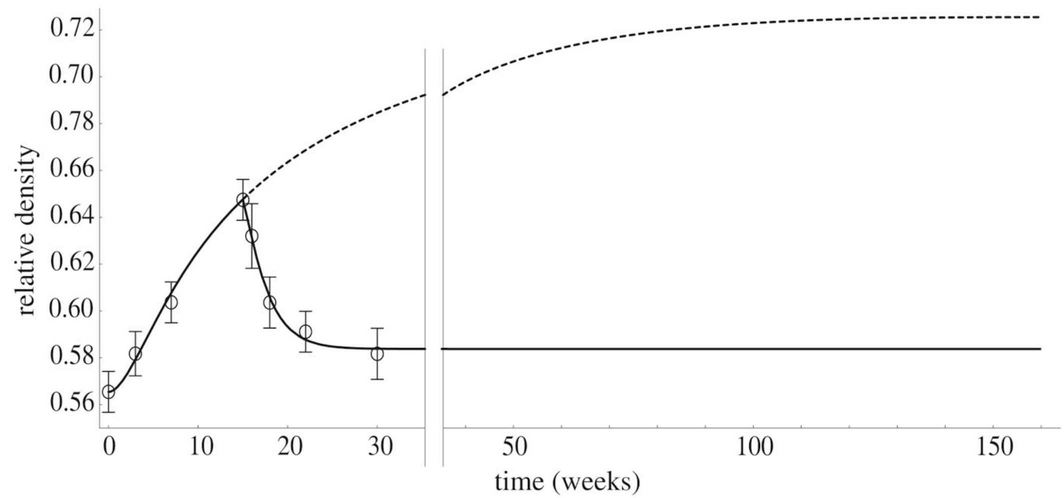
post-surgery after 1 year



J. D. Bobyn and C. A. Engh, Non-Cemented THA, Raven Press (1988)

$$\frac{\partial \rho(x,t)}{\partial t} = v(\psi(x,t) - \psi_e)$$

$$\frac{d\rho}{dt} = v\left(\frac{{\rho_c}^2}{2E_c}\frac{\sigma^2}{\rho^3} - \psi_e\right)$$



Terrier et al, Clin Biomech, 2005

ODE example: bone adaptation

$$\frac{d\rho}{dt} = v\left(\frac{A}{\rho^3} - B\right)$$

ρ : bone density (dependent variable)

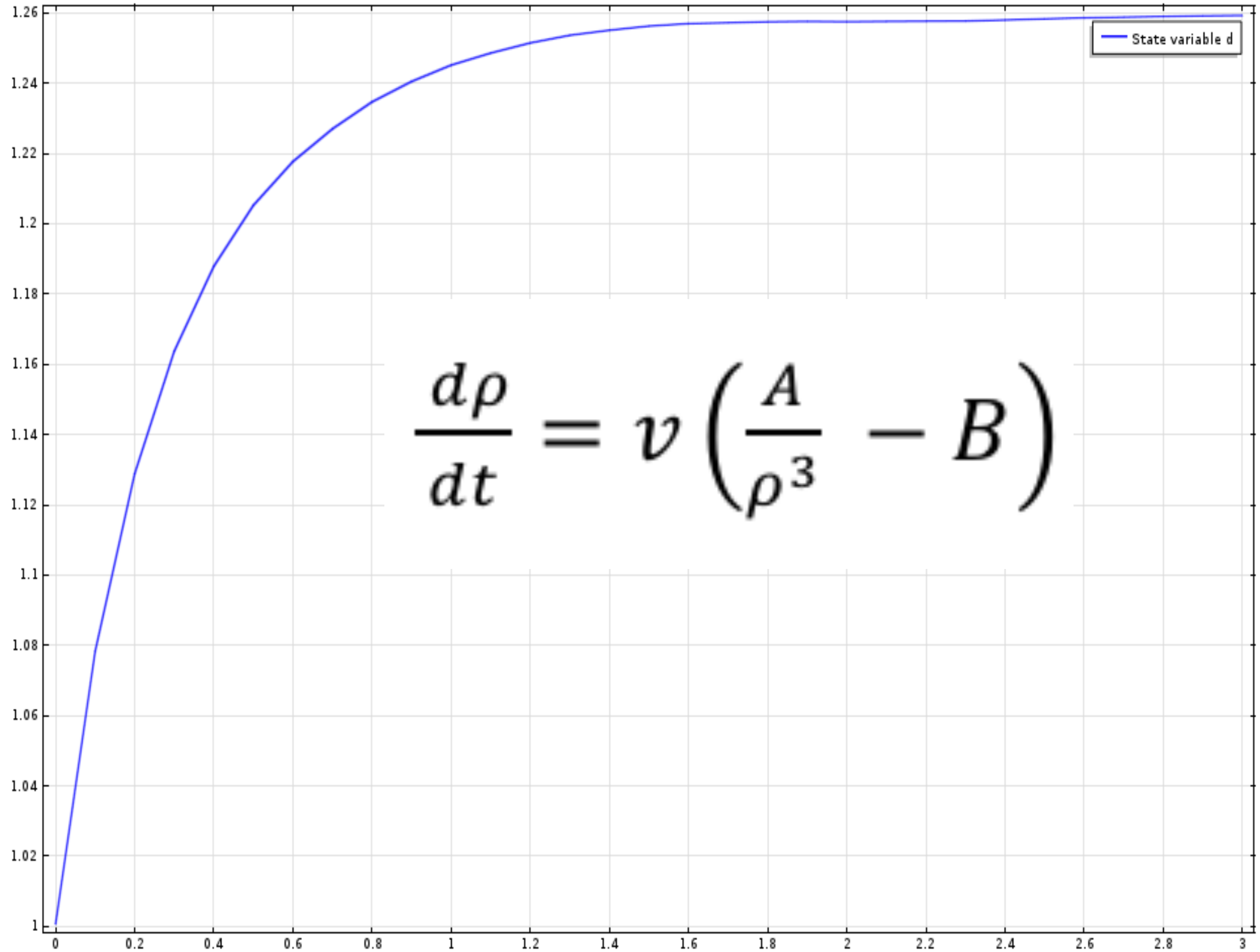
A : mechanical (actual) stimulus ($A = 2$)

B : equilibrium stimulus ($B = 1$)

v : remodeling rate ($v = 1$)

Initial value $\rho(0) = 1$

ODE example: bone adaptation



$$\frac{d\rho}{dt} = v\left(\frac{A}{\rho^3} - B\right)$$

Try with other initial conditions or constants

Partial Differential Equation (PDE)

$$F(x_1, \cdots x_n, u, \frac{\partial}{\partial x_1}u, \cdots \frac{\partial}{\partial x_n}u, \frac{\partial^2}{\partial x_1 \partial x_1}u, \frac{\partial^2}{\partial x_1 \partial x_2}u, \cdots) = 0$$

- u_i dependent variables (functions)
- x_i independent variables
  - $x_1 = t$ (time)
  - $x_2 = x, x_3 = y, x_4 = z$ (space)
- No time dependency (steady state or equilibrium)
- Existence and uniqueness not guaranteed in general, but usually locally if well-posed

Well-posed PDE

- Regular PDE and domain (Cauchy problem)
- Constitutive equations
- Boundary conditions
- Initial conditions

$\Rightarrow$ A unique & stable solution exists (locally)

Boundary conditions

- Value of the dependent variable u (and/or its derivative) on the boundary for all time t
- **Dirichlet**: u imposed on the boundary
- **Neumann**: du/dn imposed on the boundary
- Mixed: Dirichlet and Neumann on boundary parts
- Cauchy: Dirichlet and Neumann on boundary
- Robin : $u + du/dn$ imposed on the boundary

Initial conditions

- Value of the dependent variable, and/or its derivatives, at time $t = 0$, for the entire domain
- Initial value problem

$$u(x, t = 0) = u_0(x)$$

Typical PDE operators

Differential operators

- Gradient:

$$\nabla = \frac{\partial}{\partial x}\hat{\mathbf{x}} + \frac{\partial}{\partial y}\hat{\mathbf{y}} + \frac{\partial}{\partial z}\hat{\mathbf{z}}$$

- Divergence:

$$\operatorname{div} \vec{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = \nabla \cdot \vec{v}$$

- Rotation (curl):

$$\operatorname{curl} \vec{v} = \left(\frac{\partial v_z}{\partial y} - \frac{\partial v_y}{\partial z}\right)\hat{\mathbf{x}} + \left(\frac{\partial v_x}{\partial z} - \frac{\partial v_z}{\partial x}\right)\hat{\mathbf{y}} + \left(\frac{\partial v_y}{\partial x} - \frac{\partial v_x}{\partial y}\right)\hat{\mathbf{z}} = \nabla \times \vec{v}$$

- Laplacian:

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla \cdot \nabla = \nabla^2$$

PDE: scalar coefficient form

$$e_a \frac{\partial^2 u}{\partial t^2} + d_a \frac{\partial u}{\partial t} + \nabla \cdot (-c\nabla u - \boldsymbol{\alpha} u + \gamma) + \beta \cdot \nabla u + au = f \qquad \text{in } \Omega$$

$$\mathbf{n} \cdot (c\nabla u + \alpha u - \gamma) + qu = g - h^T \mu \quad \text{(Generalized Neumann) on } \partial\Omega$$

$$u = r \quad \text{(Generalized Dirichlet) on } \partial\Omega$$

- Coefficients (c, α, γ, β, a, h) and f, g, and r can depend on x, y, z, t
- PDE is linear when coefficients depend only on (x, y, z), or constant
- PDE is nonlinear if coefficients depend on u (or its derivatives)
- **Initial condition is required**

Partial Differential Equation (PDE)

Most physical PDE are 2nd order, with linear coef.

- Elliptic: solid, heat (steady state) $$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} = 0$$
- Parabolic: heat, diffusion $$\frac{\partial w}{\partial t} - \frac{\partial^2 w}{\partial x^2} = 0$$
- Hyperbolic: wave, advection $$\frac{\partial^2 w}{\partial t^2} - \frac{\partial^2 w}{\partial x^2} = 0$$

Example of elliptic PDE

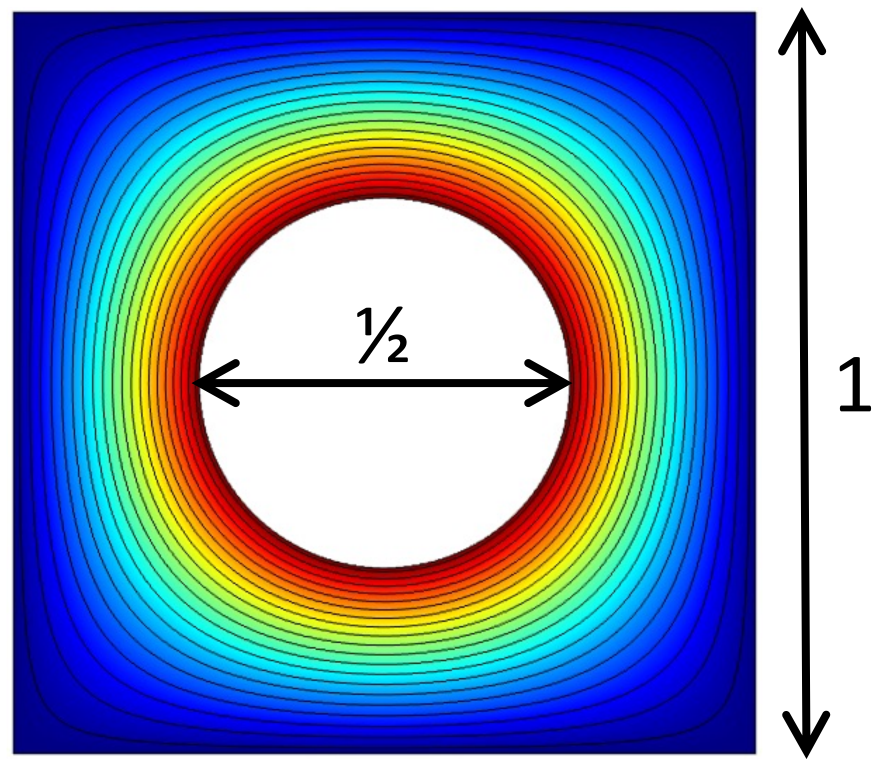
- Laplace equation $\nabla \cdot (\nabla u) = 0$
- Static solid deformation (displacement u)
- Static heat equation (temperature u, heat flux du/dx)
  - Dirichlet: Fixed temperature (u) on boundary
  - Neumann: Fixed heat flux (insolation) on boundary
- Electromagnetism, astronomy, fluid dynamics

Example of elliptic PDE

- 2D Laplace on a square domain with a hole
- $u_{xx} + u_{yy} = 0$
- Dirichlet conditions

  $u = 1$ (int. circle)

  $u = 0$ (ext. frame)

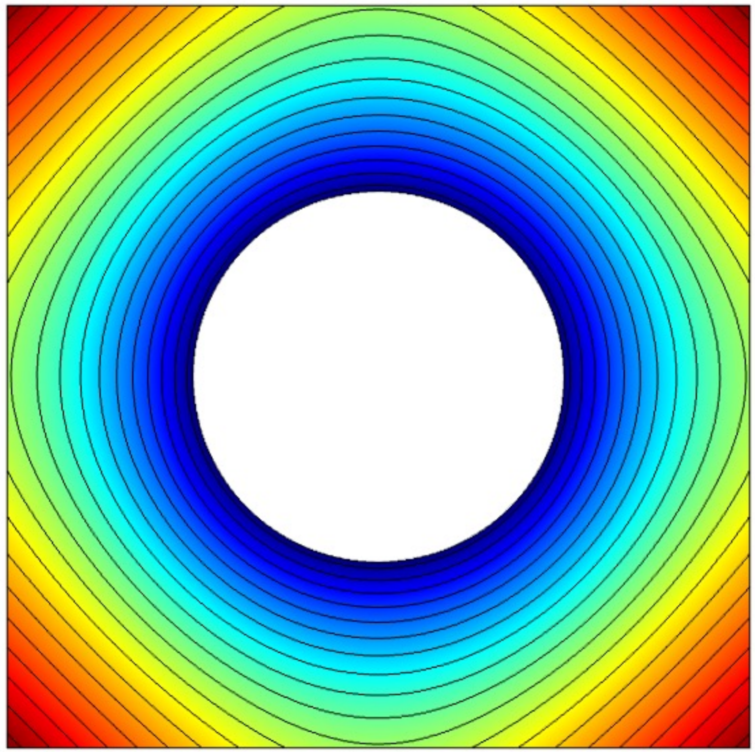


Example of elliptic PDE

- 2D Laplace on a square domain with a hole
- $u_{xx} + u_{yy} = 0$
- Mixed (Dirichlet + Neumann)

  $u = 1$ (int. circle)

  $du/dn = 1$ (ext. frame)



Example of parabolic PDE

Equation of heat

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \cdot \nabla T = \nabla \cdot (k \nabla T) + Q$$

Convective term   Diffusive term

ρ is the density (SI unit: kg/m^3)

C_p is the specific heat capacity at constant pressure (SI unit: J/(kg·K))

T is absolute temperature (SI unit: K)

$\mathbf{u}$ is the velocity vector (SI unit: m/s)

k is the thermal conductivity (SI unit: W/(m·K))

Q contains heat sources other than viscous heating (SI unit: W/m^3)

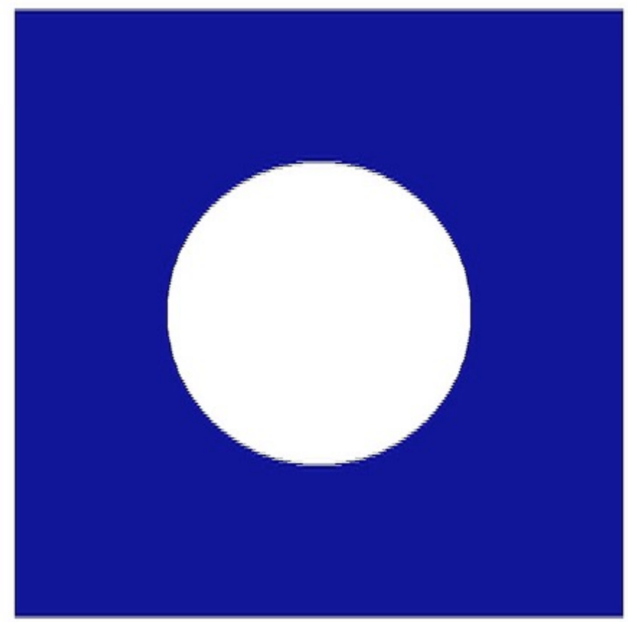
Example of parabolic PDE

- Parabolic heat equation $d_a \frac{\partial u}{\partial t} - \nabla \cdot (c \nabla u) = f$
- No source $f = 0$
- Evolution of $u(t)$, $t \in [0, 0.1]$

$u(t_0) = 0$

$du/dn = 1$ (int. circle)

$u = 0$ (ext. frame)



Well-posed problem

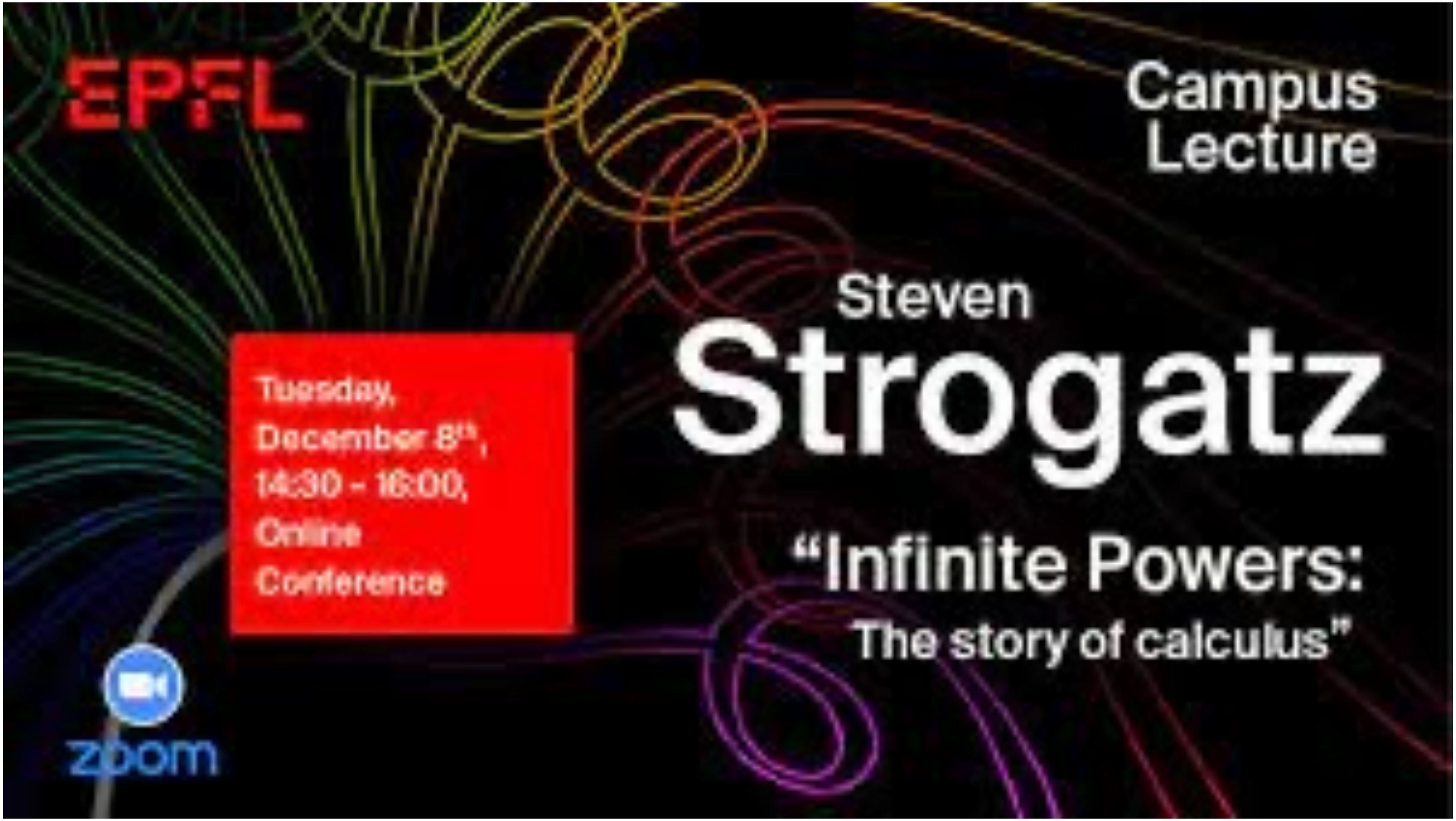
- Domain (geometry)
- PDE (physics)
- Constitutive laws (material)
- Initial conditions
- Boundary conditions

Summary

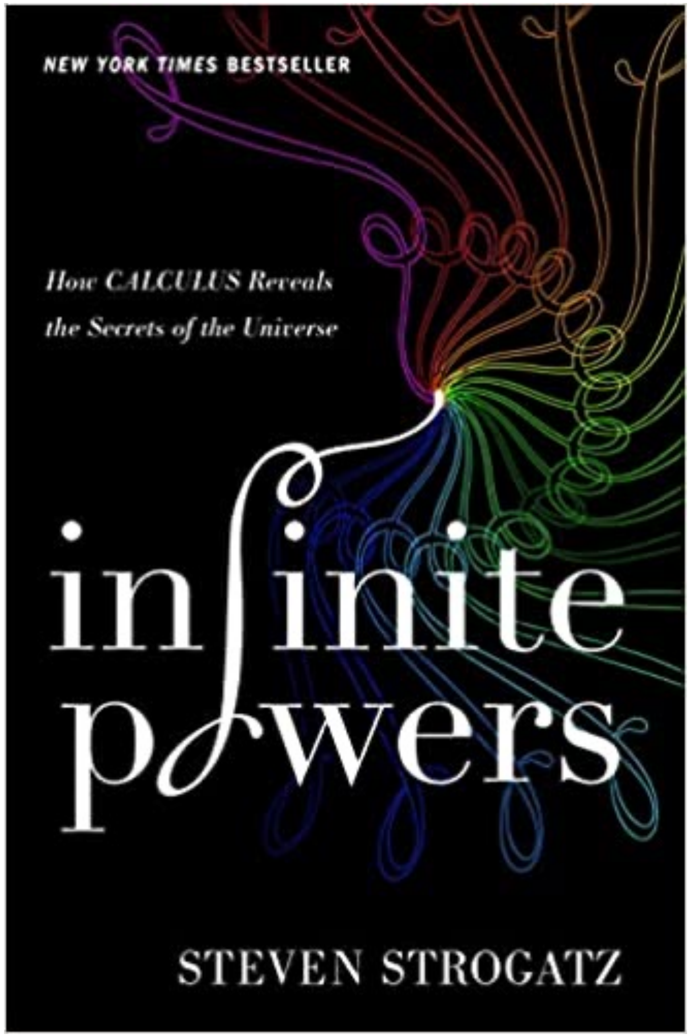
- Most biomechanical (bioengineering) systems (problems) can be represented by Partial Differential Equations (PDEs)
- Well-posed PDEs have a unique solution
- Most PDEs can’t be solved analytically
- Many PDEs can be solved by numerical methods
- Some PDEs can’t be solved by numerical methods

Sophus Lie (1842-1899)

"Among all of the mathematical disciplines,
the theory of differential equations is the most important…
It furnishes the explanation of all those elementary
manifestations of nature which involve time."



https://www.youtube.com/watch?v=3xP19pqUGlw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Comment le calcul infinitésimal révèle les secrets de l'univers

References

- Partial Differential Equations I, Basic Theory, Michael E. Taylor
- Partial Differential Equations II, Qualitative Studies of Linear Equations, Michael E. Taylor
- Partial Differential Equations III, Nonlinear Equations, Michael E. Taylor
- Partial Differential Equations, Emmanuele DiBenedetto
- Partial Differential Equations, Modeling and Numerical Simulation, Roland Glowinski and Pekka Neittaanmäki
- Linear Partial Differential Equations for Scientists and Engineers, Tyn Myint-U and Lokenath Debnath
- Partial Differential Equations, Laurence C Evans

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