Numerical approximation for PDEs

Introduction to numerical simulation

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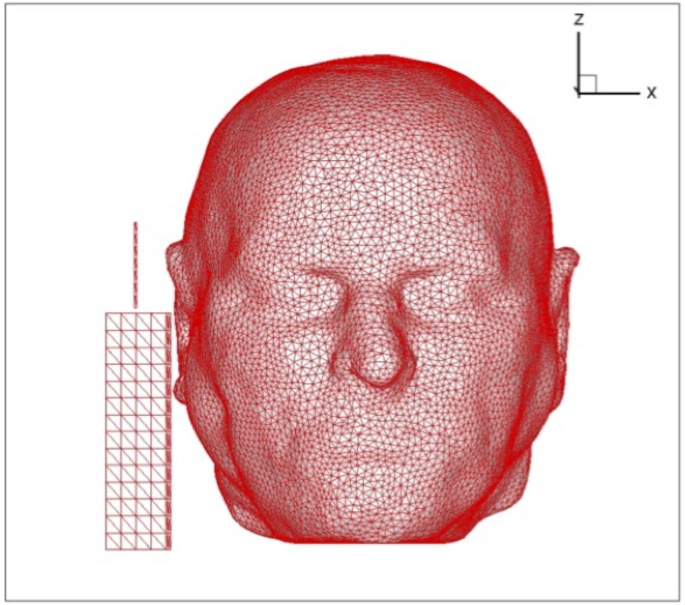
Mathematical modelling and numerical simulation

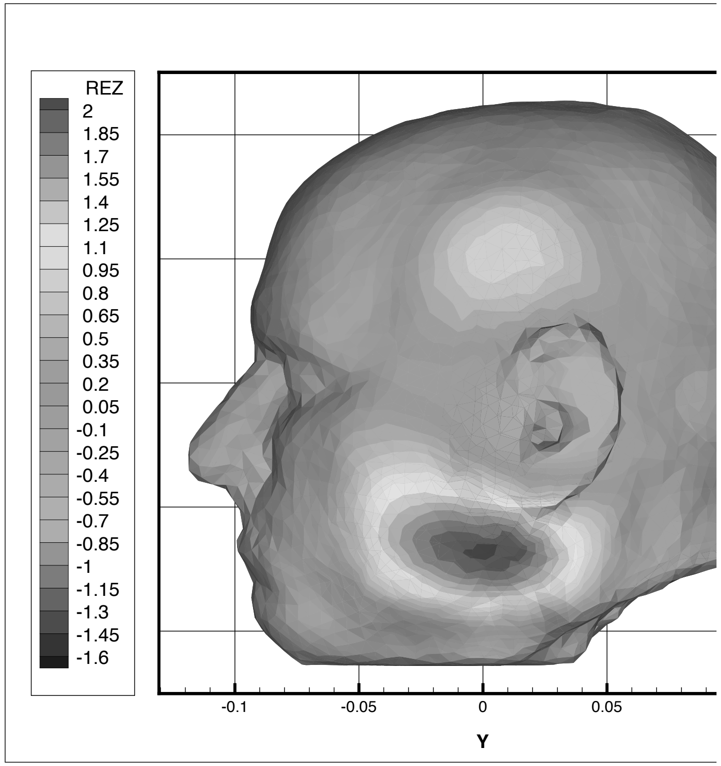
- Mathematical modelling
- Mathematical and numerical analysis of models
- Numerical simulation

- Numerous fields of applications:
- Engineering: mechanics, electromagnetism, geoseismics, robotics
- Other fields of science: physics, biology, chemistry…
- Numerous new problems arise each year (medicine, environment, climate etc…)

Electromagnetic waves

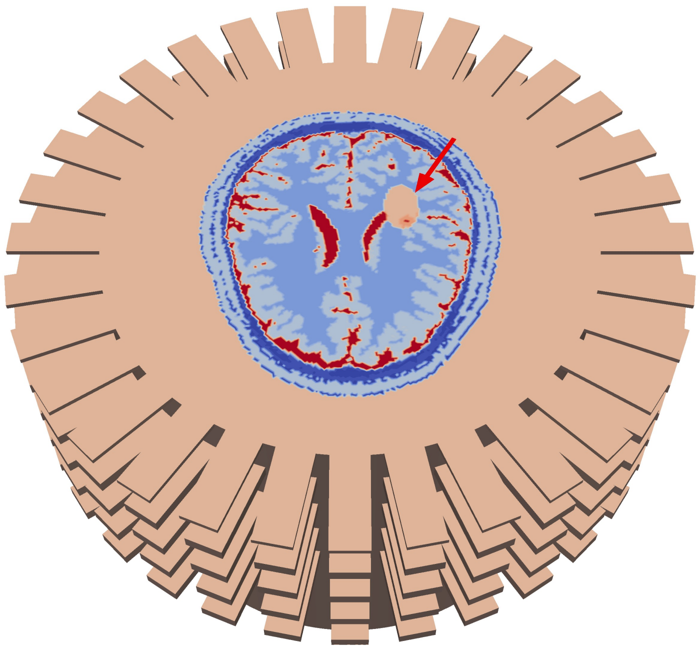
- Mobile phones

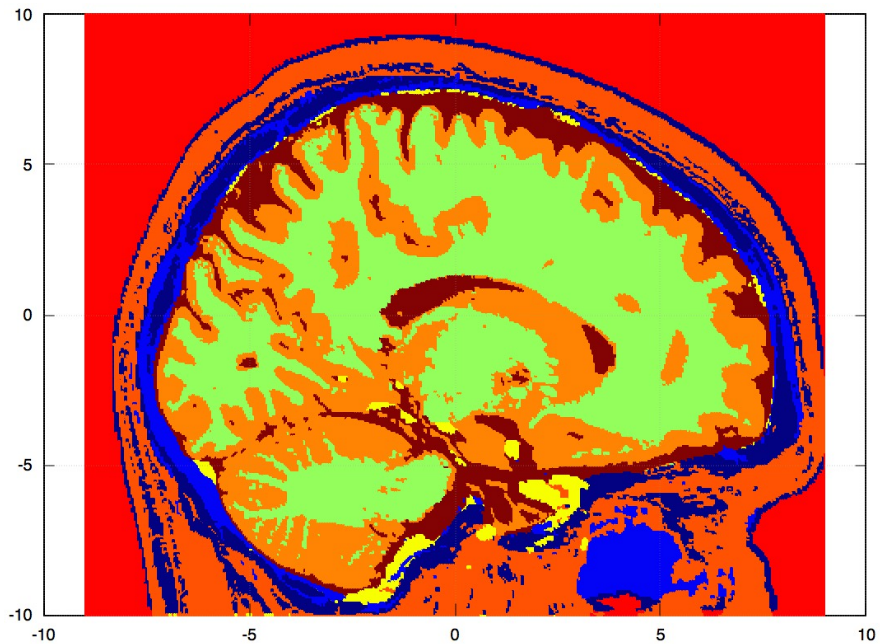




Medical imaging

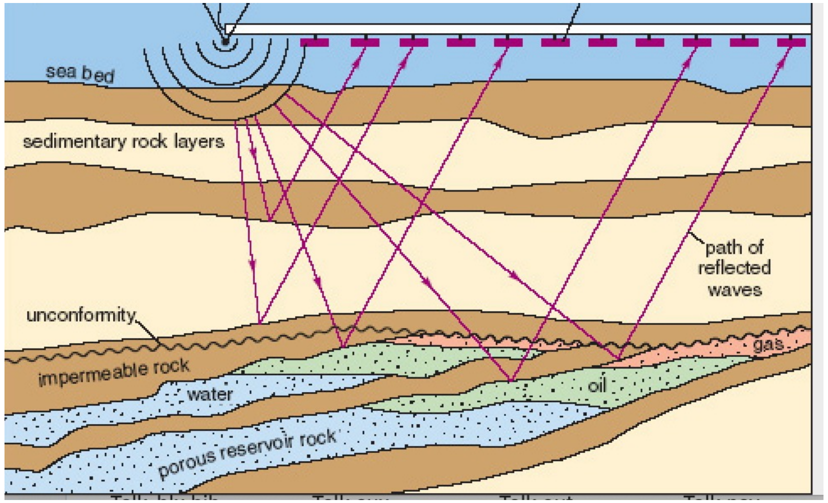
- Reconstruct electrical properties of the brain

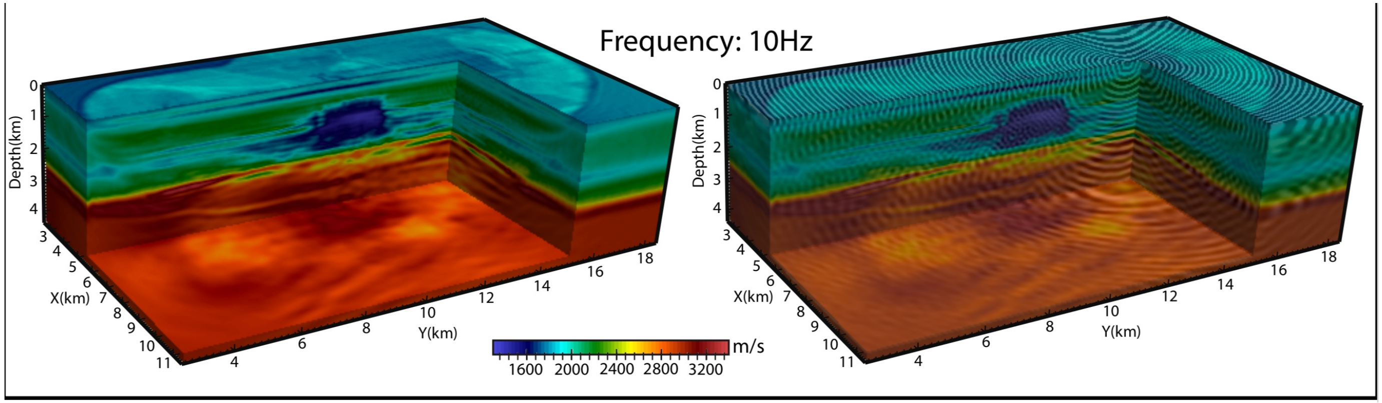




Seismic imaging

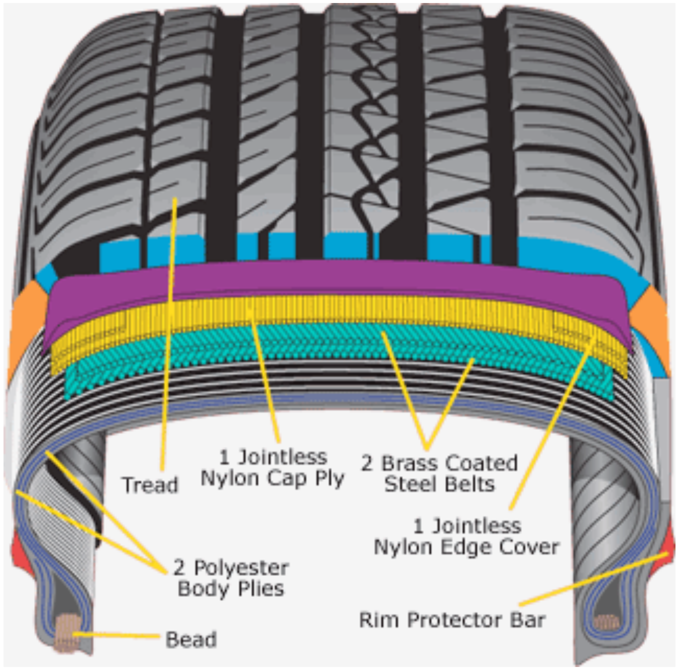
- Reconstruct subsurface properties from measures





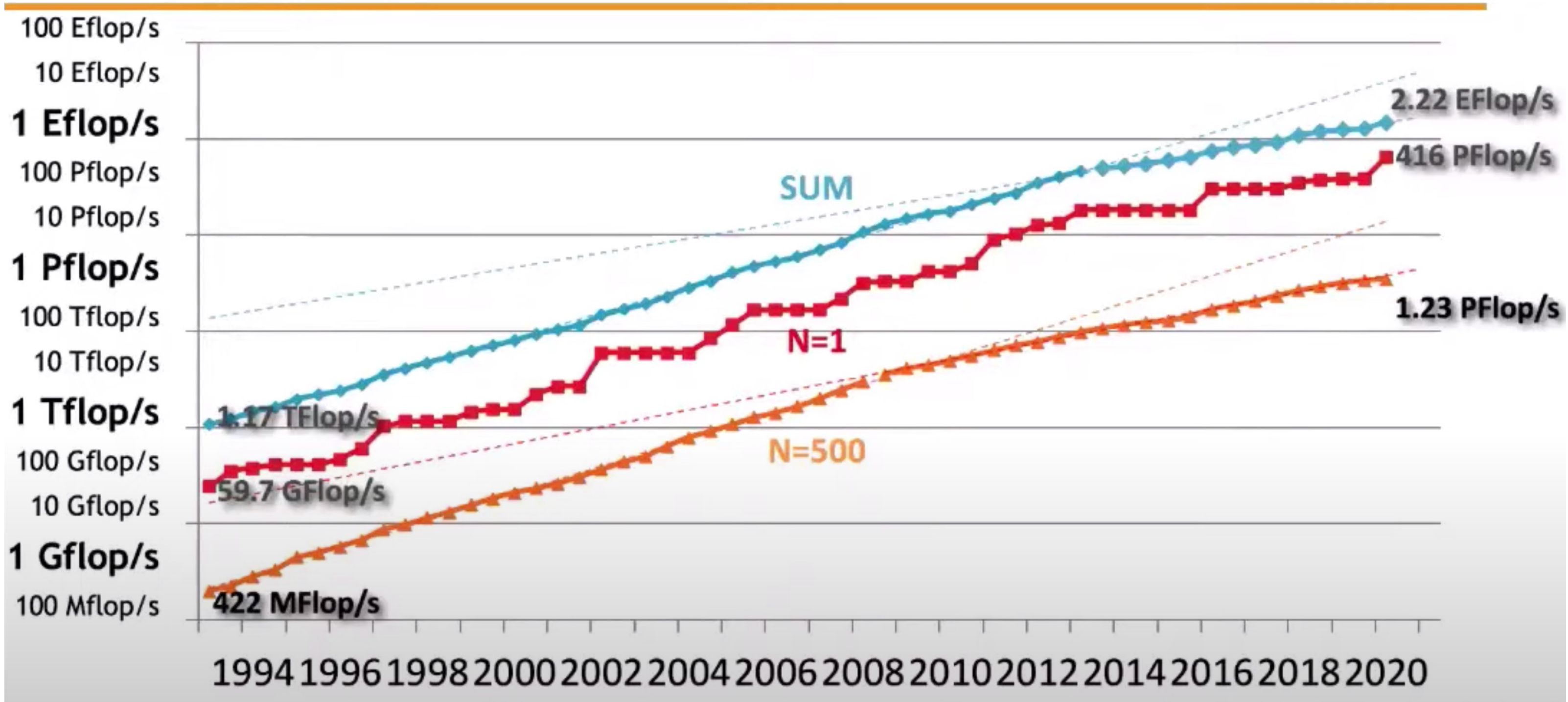
Computational mechanics

- A tire is a complex material with a multiscale structure.
- Mathematical model: non-linear elasticity



Developpement of Applied Maths

- Their development explose because of powerful computers



Moore’s law

Exponential growth of computer power

- 1976 - Cray 1 (USA): 133 Mflops
- 1993 - Thinking Machine CM5 (USA): 59,700 Mflops (59 Gflops)
- 2005-2006 - IBM BlueGene (USA): 280,600,000 Mflops (280 Tflops)
- 2008 - IBM Roadrunner : 1,105,000,000 Mflops (1 Pflops) 129,600 processeurs (de PlayStation !)
- 2011 - K computer (Japon): 10,510,000,000 Mflops (10.5 Pflops)
- 2015 - Tianhe-2 (Chine): 33,860,000,000 Mflops (33.8 Pflops)
- 2018 - Summit - IBM (USA): 122,300,000,000 Mflops (122 Pflops),

Objectives of the lecture

- Acquire the (first) mathematical and numerical tools to carry out, understand and interpret numerical simulations

Purpose:

- Weather prediction, environment, safety ...
- Design and optimization.
- Experimentation: validation of a model, verification of a theory ...

Mathematics has become an experimental science!

Outline of today's lecture

- Explain what is mathematical modelling (about numerical modelling next week).
- Give an example of the simplest mathematical model (convection-diffusion equation)
- Define partial differential equations.
- Classify these equations and present their qualitative properties.
- Prove some important properties on well-chosen examples.

Remark: we don't really do mathematical analysis at this stage.

Example of modelling: convection-diffusion

- Unknown function: $\theta(t, \boldsymbol{x}), t \in R^+, \boldsymbol{x} \in R^n$ (t – time, $\boldsymbol{x}$ – space variable)
- Gradient (in space)

$$\nabla\theta = \left(\frac{\partial\theta}{\partial x_1}, \dots, \frac{\partial\theta}{\partial x_N}\right)^T$$

- Divergence

$$q = (q_1, \dots, q_N)^T: \qquad \operatorname{div} q = \sum_{i=1}^{N} \frac{\partial q_i}{\partial x_i}$$

- Laplace operator

$$\Delta\theta = \operatorname{div}(\nabla\theta) = \sum_{i=1}^{N} \frac{\partial^2\theta}{\partial x_i^2}$$

Application of physical laws

- Physical quantities: temperature θ, heat flux q, thermic source term f, a physical constant $c > 0$.
- Application of a physical law: in a general elementary volume V:

Variation in time = sources + losses or entries through the walls

$$\frac{d}{dt}\left(\int_V c\,\theta\,dx\right) = \int_V f\,dx - \int_{\partial V} q\cdot n\,ds.$$

- Application of Gauss' theorem (or divergence theorem):

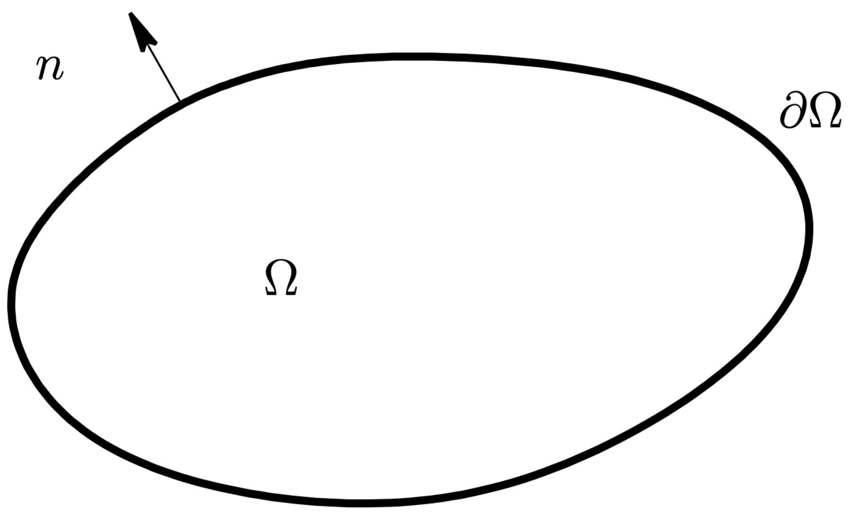
$$\int_{\partial V} q\cdot n\,ds = \int_V \operatorname{div} q\,dx.$$

- We permute the derivative in time and the integral over V. The volume V is arbitrary

$$c\frac{\partial\theta}{\partial t} + \operatorname{div} q = f$$

Computational domain and unit normal

- By convention, the normal to the boundary is outward and $||\boldsymbol{n}|| = 1$
- Notation for the boundary $\partial\Omega$



Constitutive laws (Fourier or Fick)

Fick's law: linear relationship between *the flux across a surface (q)* and *convection along velocity (V) + diffusion along the opposite of thermal gradient*.

$$q(t, x) = c\,V\,\theta(t, x) - k\,\nabla\theta(t, x)$$

- Physical quantities: convective speed *V* and thermal conductivity $k > 0$.

Additional relations

- **Initial conditions (IC)**: $\theta(t = 0, x) = \theta_0(x)$
- **Boundary conditions (BC)**:
  - *Dirichlet*: $\theta(t, x) = 0, \partial\Omega$ (thermostat = the temperature is maintained fixed)
  - *Neumann*: $q(t, x) = 0, \partial\Omega$ (adiabatic = the heat flux is maintained constant)

Convection diffusion-model

- Mathematical model given by a *partial differential equation* (PDE)

$$
\begin{cases}
c\dfrac{\partial \theta}{\partial t} + c\,V\cdot\nabla\theta - k\Delta\theta = f & \text{dans } \Omega\times\mathbb{R}_*^+ \\
\theta = 0 & \text{sur } \partial\Omega\times\mathbb{R}_*^+ \\
\theta(t=0,x) = \theta_0(x) & \text{dans } \Omega
\end{cases}
$$

- *Data*: $c, V, k, f(t,x), \theta_0(x), \Omega$.
- *Unknown function*: $\theta(t,x)$.

Remark: we have used only physical laws to derive the model!

More mathematical modelling

- Balance between the convection term and the diffusion term measured by a dimensionless quantity: the Péclet number

$$\mathrm{Pe} = \frac{cVL}{k},$$

- where L is a characteristic length (e.g. the diameter of the domain).
- Further simplifications:

$\mathrm{Pe} << 1 \quad \Rightarrow$ Heat equation

$\mathrm{Pe} >> 1 \quad \Rightarrow$ Advection equation

- We end up with hree different models (heat, advection, advection-diffusion)!

Simplified models

The heat equation ($\mathrm{Pe} = 0$):

$$\begin{cases} c\dfrac{\partial \theta}{\partial t} - k\Delta\theta = f & \text{dans } \Omega \times \mathbb{R}_*^+ \\ \theta = 0 & \text{sur } \partial\Omega \times \mathbb{R}_*^+ \\ \theta(t=0,x) = \theta_0(x) & \text{dans } \Omega \end{cases}$$

The advection equation ($\mathrm{Pe} = \infty$):

$$\begin{cases} c\dfrac{\partial \theta}{\partial t} + c\,V \cdot \nabla\theta = f & \text{dans } \Omega \times \mathbb{R}_*^+ \\ \theta = 0 & \text{sur } \{x \in \partial\Omega \text{ tel que } V \cdot n(x) < 0\} \times \mathbb{R}_*^+ \\ \theta(t=0,x) = \theta_0(x) & \text{dans } \Omega \end{cases}$$

Explicit solutions – 1d case

- Simplified case: $\Omega = R$ (no BC), source term $f = 0, \nu = \frac{k}{c}$
- *Covection diffusion equation*

$$\theta(t,x) = \frac{1}{\sqrt{4\pi\nu t}} \int_{-\infty}^{+\infty} \theta_0(y) \exp\left(-\frac{(x - Vt - y)^2}{4\nu t}\right) dy.$$

- *Heat equation*

$$\theta(t,x) = \frac{1}{\sqrt{4\pi\nu t}} \int_{-\infty}^{+\infty} \theta_0(y) \exp\left(-\frac{(x - y)^2}{4\nu t}\right) dy.$$

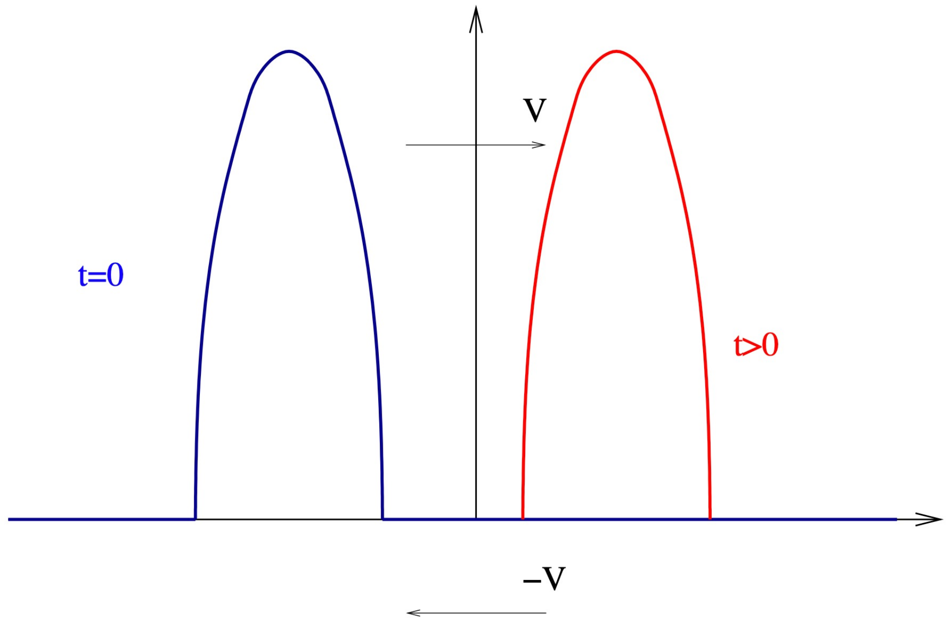
- *Advection equation*:

$$\theta(t,x) = \theta_0(x - Vt).$$

Properties – convection equation

- **Maximum principle** verified by the solution $\theta(t, x) = \theta_0\,(x - Vt)$

$$\min \theta_0(x) \leq \theta(t, x) \leq \max \theta_0(x)$$



Properties – heat and convection-diffusion

- **Maximum principle** for the explicit solutions of the heat and convection-diffusion equations
- Solution = convolution between the initial condition and a Gaussian kernel

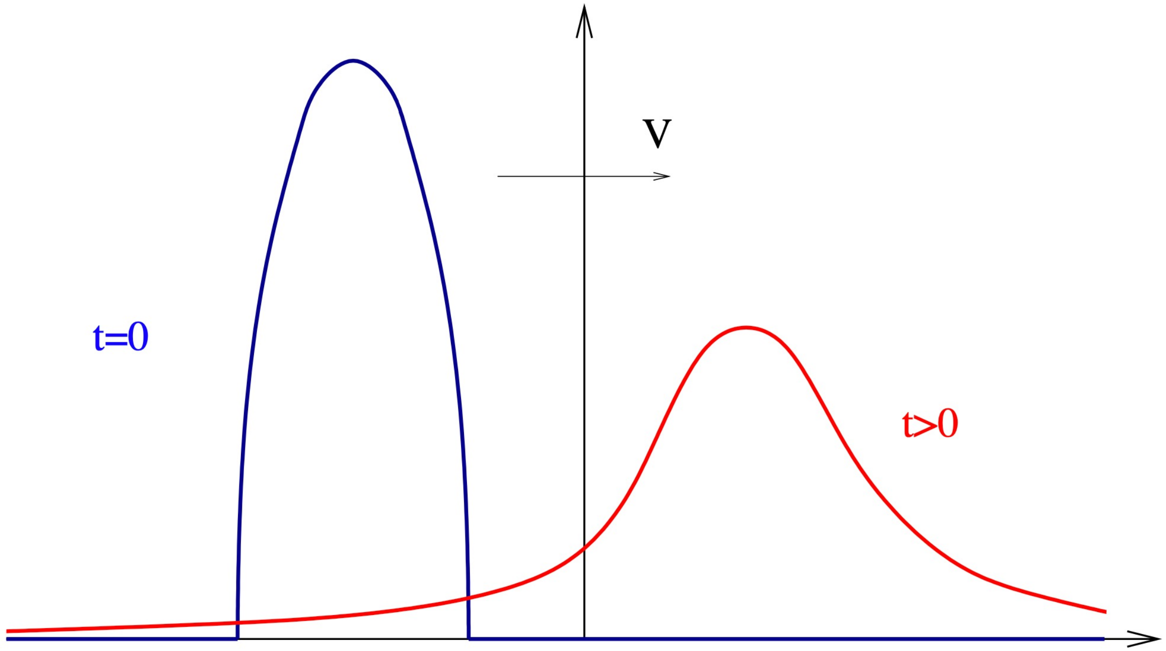
$$\frac{1}{\sqrt{4\pi\nu t}}\int_{-\infty}^{+\infty}\exp\left(-\frac{(x-Vt-y)^2}{4\nu t}\right)dy=1.$$

- **Infinite propagation speed**:

if $\theta_0(x)\geq 0, \theta_0\neq 0 \;\Rightarrow \theta(t,x)>\; 0\;\forall t>0.$

Solution of the convection-diffusion equation

- Convolution of the initial condition with a Gaussian kernel.



Analysis of the mathematical models

- **Maximum principle** for the three models

$$\min_{x\in\mathbb{R}} \theta_0(x) \leq \theta(x,t) \leq \max_{x\in\mathbb{R}} \theta_0(x)$$

- (i)**Reversibility**: the advection equation is "reversible" in time but heat and convection-diffusion are irreversible.

- **Propagation speed**: finite for the advection equation, infinite for the heat and convection-diffusion equation.

A few remarks

- The same equation (convection-diffusion or heat equation) can model very different phenomena: option pricing in finance, concentration of a pollutant, fluid flows, electrostatics, etc…
- There are a lot of models based on partial differential equations (PDE): linear elasticity, Navier-Stokes equations, Maxwell's equations, etc..
- PDEs can be classified according to their intrinsic and qualitative properties.

Well posed boundary value problem

- *Boundary value problem* = PDE with boundary conditions on the entire domain boundary.
- *Cauchy problem* = PDE where, for the time variable t, the “boundary” conditions are initial (and not final) conditions.
- We say that the problem A(u) = f *is well posed in the sense of Hadamard* if for any given f it admits a unique solution u, and if this solution u continuously depends on the given f.
- Necessary condition to do numerical computations!
- Small variations in f (measurement or rounding errors) should only lead to small variations in u.