# Differentiaal Vergelijkingen In de Aardwetenschappen

## PDEs - chapt 13 - diffusion equation

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## the diffusion equation (1)

The heat transport equation writes :

$$\rho c_p \left( \frac{\partial T}{\partial t} + \underbrace{\mathbf{v} \cdot \boldsymbol{\nabla} T}_{adv.} \right) = \underbrace{\boldsymbol{\nabla} \cdot (k \boldsymbol{\nabla} T)}_{diff.} + \underbrace{H}_{prod.}$$

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Then the temperature field must verify :

$$\rho c_p \frac{\partial T}{\partial t} = \boldsymbol{\nabla} \cdot (k \boldsymbol{\nabla} T)$$

If $k = constant$ , then it is equivalent to solve

$$\frac{\partial T}{\partial t} = \alpha^2 \boldsymbol{\nabla}^2 T$$

where $\alpha^2 = k / \rho c_p$ is the heat diffusivity.

## the diffusion equation (2)

Partial separation of variables into a space equation and a time equation :

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- the left side is a function of time $t$
- the right side is a function only of the space variables $x, y, z$

$\rightarrow$ both sides are the same constant

# the diffusion equation (3)

We obtain

$$\begin{aligned} \frac{1}{\alpha^2}\frac{1}{\Phi}\frac{\partial \Phi}{\partial t} &= -k^2 \\ \frac{1}{\theta}\nabla^2\theta &= -k^2 \end{aligned}$$

or,

$$\frac{\partial \Phi}{\partial t} + k^2\alpha^2\Phi = 0 \quad (1)$$

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Eq(2) is the Helmholtz equation.
Eq(1) can be integrated :

$$\Phi(t) = e^{-k^2\alpha^2 t}$$

(as $t$ increases the temperature of a body cannot increase to infinity)

# Maths, hairstyle and history (continued)

Hermann Ludwig Ferdinand von Helmholtz (1821-1894)
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*Whoever in the pursuit of science, seeks after immediate practical utility may rest assured that he seeks in vain.*

# Helmholtz Resonators (1)

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- These resonators were developed for picking out particular frequencies from a complex sound.
- They consists of a body to contain a volume of air, a hole or neck in which a slug of air can vibrate back and forth, and a slender nipple that can be held in the ear canal (or, today, connected to a sound level meter).
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http ://physics.kenyon.edu/EarlyApparatus/Rudolf_Koenig_Apparatus/Helmholtz_Resonator/Helmholtz_Resonator.html

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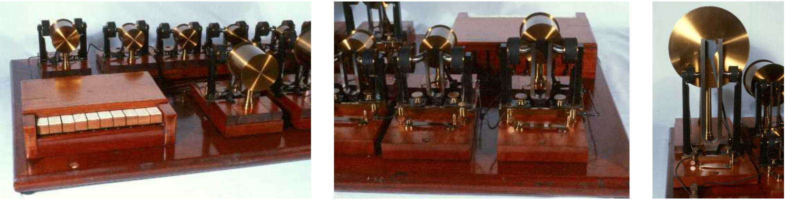

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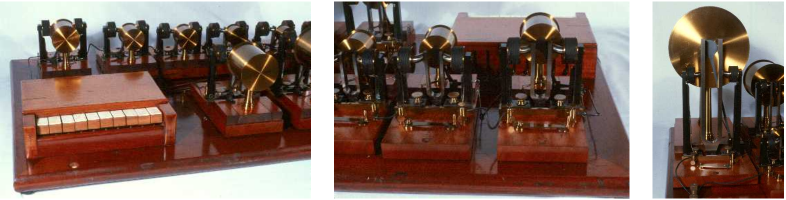

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- The ten electrically-driven tuning forks, each facing a Helmholtz resonator tuned to the same frequency, run continuously, but produce little sound.
- Pressing one of the keys moves the dull black shutter away from the hole of the resonator, and the sound becomes quite loud.
- Rubber feet under the corners of the wooden stand keep the vibrations from reaching the baseplate that runs under all ten of the tuning fork systems.

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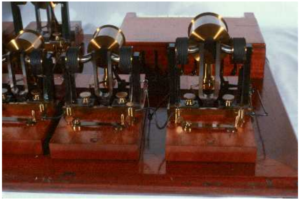
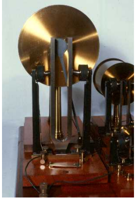

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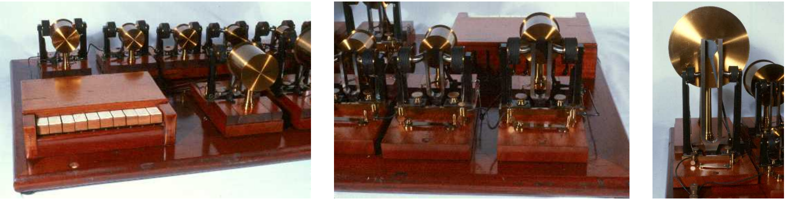

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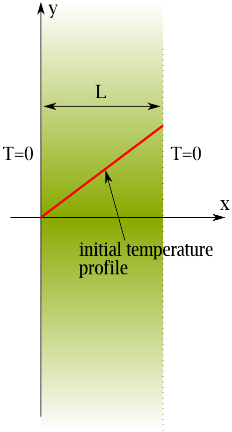
# the diffusion equation - Example (1)

Let us consider a flow of heat through a slab of thickness $L$ :

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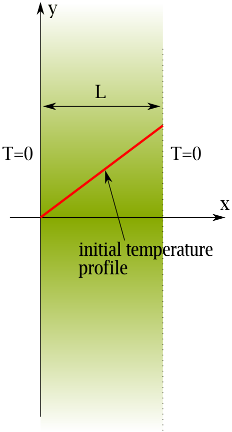


The slab has initially a steady-state temperature distribution with $T = 0$ at $x = 0$ and $T = 100$ at $x = L$.
The faces of the slab are so large that we neglect end effects.
Heat flows only in the $x$ direction

# the diffusion equation - Example (2)

We want to find the temperature for $x \in [0, L]$ at all times.
We need to solve :

$$\frac{d^2\theta}{dx^2} + k^2\theta = 0$$

which leads to

$$\theta(x) = \left\{ \begin{array}{l} \sin kx \\ \cos kx \end{array} \right.$$

and the general solution writes

$$T(x,t) = \theta(x)\Phi(t) = \left\{ \begin{array}{c} \sin kx \\ \cos kx \end{array} \right\} e^{-k^2\alpha^2 t}$$

# the diffusion equation - Example (3)

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- we impose $T(L,t) = 0$ which leads to

$$k = n\pi/L$$

The basis functions are then

$$T_n(x,t) = e^{-(n\pi\alpha/L)^2 t} \sin \frac{n\pi x}{L}$$

The solution to the problem writes :

$$T(x,t) = \sum_{n=1}^{\infty} b_n T_n(x,t) = \sum_{n=1}^{\infty} b_n e^{-(n\pi\alpha/L)^2 t} \sin \frac{n\pi x}{L}$$

# the diffusion equation - Example (4)

Finally, at $t = 0$, we want $T(x, 0) = 100x/L$ :

$$\frac{100}{L}x = \sum_{n=1}^{\infty} b_n \sin \frac{n\pi x}{L}$$

This means finding the fourier sine series for function $100x/L$ on $[0, L]$. We arrive at

$$b_n = \frac{200}{\pi} \frac{(-1)^{n-1}}{n}$$

and then

$$T(x, t) = \frac{200}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} e^{-(n\pi\alpha/L)^2 t} \sin \frac{n\pi x}{L}$$

# Numerical approach (1)

Use ELEFANT code to solve the same problem.

Programming the analytical solution

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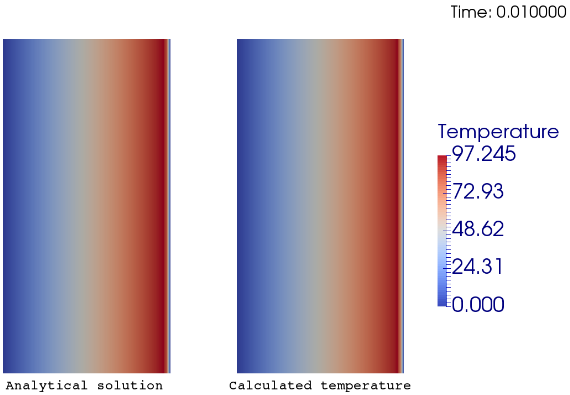
```
tt=0
do n=1,100
tt=tt+((-1)**(n-1))/dble(n) * exp(-time*(n*pi/Lx)**2)*sin(n*pi*x/Lx)
end do
tt=tt*200.d0/pi
```

# Numerical approach (2)

film

# Numerical approach (3)



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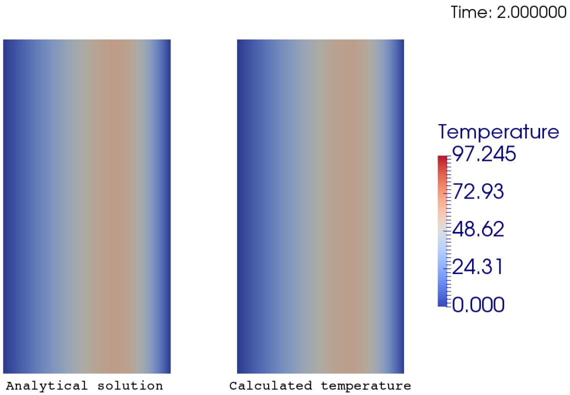

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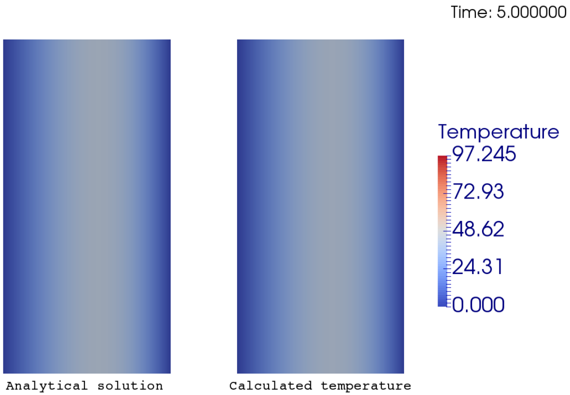

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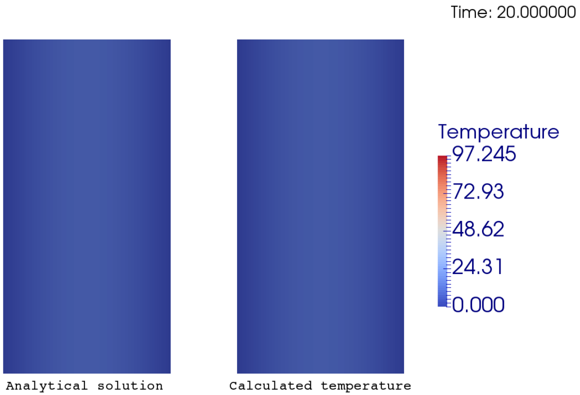

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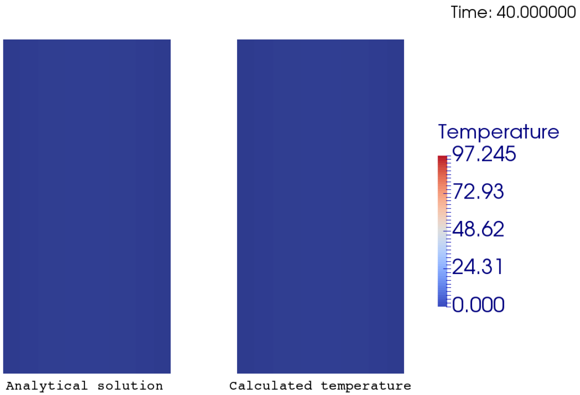
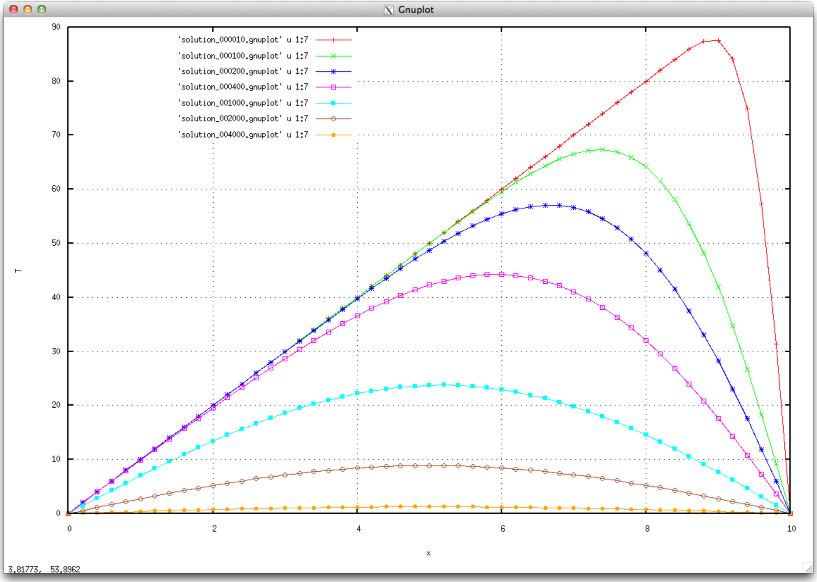


# Numerical approach (4)



## The Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

This is the wave equation in quantum mechanics.

- $\hbar$ : Planck's constant (divided by $2\pi$). $h = 6.626070040 \times 10^{34}$
- $m$ : mass of a particle
- $V$ : potential energy of the particle
- the function $\Psi$ is complex and its absolute square $|\Psi|^2$ is proportional to the position probability of the particle.

# Maths, hairstyle and history (continued)

Erwin Rudolf Josef Alexander Schrödinger (1887-1961)
Austrian born physicist and theoretical biologist
Nobel Prize in Physics in 1933

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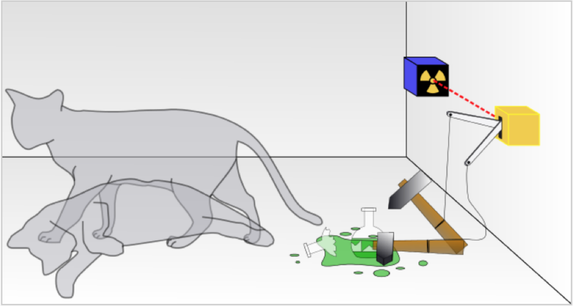
*"I do not like quantum mechanics,*
*and I am sorry I ever had anything to do with it."*

*"Anyone who is not shocked by quantum theory has not understood it."*
Niels Bohr

*"If you think you understand quantum mechanics, you don't understand quantum mechanics."*
Richard Feynman

# Schrödinger's cat



Schrödinger's cat: a cat, a flask of poison, and a radioactive source are placed in a sealed box. If an internal monitor detects radioactivity (i.e., a single atom decaying), the flask is shattered, releasing the poison that kills the cat. The Copenhagen interpretation of quantum mechanics implies that after a while, the cat is *simultaneously* alive *and* dead. Yet, when one looks in the box, one sees the cat *either* alive *or* dead, not both alive *and* dead. This poses the question of when exactly quantum superposition ends and reality collapses into one possibility or the other.

# The Schrödinger equation (2)

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

We separate space and time variables as follows :

$$\Psi = \phi(x, y, z)\,T(t)$$

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The time equation writes

$$\frac{\partial T}{\partial t} + i\frac{ET}{\hbar} = 0$$

and we can integrate to obtain

$$T(t) = e^{-iEt/\hbar}$$

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The time-independent Schrödinger equation is then

$$-\frac{\hbar^2}{2m}\nabla^2\phi + V\phi = E\phi$$

# The Schrödinger equation (3)

Time-independent Schrödinger equation :

3. ***Quantisierung als Eigenwertproblem;***
***von E. Schrödinger.***

(Erste Mitteilung.)

§ 1. In dieser Mitteilung möchte ich zunächst an dem einfachsten Fall des (nichtrelativistischen und ungestörten) Wasserstoffatoms zeigen, daß die übliche Quantisierungsvorschrift sich durch eine andere Forderung ersetzen läßt, in der kein Wort von „ganzen Zahlen“ mehr vorkommt. Vielmehr ergibt sich die Ganzzahligkeit auf dieselbe natürliche Art, wie etwa die Ganzzahligkeit der *Knotenzahl* einer schwingenden Saite. Die neue Auffassung ist verallgemeinerungsfähig und rührt, wie ich glaube, sehr tief an das wahre Wesen der Quantenvorschriften.

Die übliche Form der letzteren knüpft an die Hamiltonsche partielle Differentialgleichung an:

$$H\left(q, \frac{\partial S}{\partial q}\right) = E \,. \tag{1}$$

Es wird von dieser Gleichung eine Lösung gesucht, welche sich darstellt als *Summe* von Funktionen je einer einzigen der unabhängigen Variablen $q$.

Wir führen nun für $S$ eine neue unbekannte $\psi$ ein derart, daß $\psi$ als ein *Produkt* von eingriffigen Funktionen der einzelnen Koordinaten erscheinen würde. D. h. wir setzen

$$S = K \lg \psi \,. \tag{2}$$

Die Konstante $K$ muß aus dimensionellen Gründen eingeführt werden, sie hat die Dimension einer *Wirkung*. Damit erhält man

$$H\left(q, \frac{K}{\psi}\frac{\partial \psi}{\partial q}\right) = E \,. \tag{1'}$$

Wir suchen nun *nicht* eine Lösung der Gleichung (1′), sondern wir stellen folgende Forderung. Gleichung (1′) läßt sich bei Vernachlässigung der Massenveränderlichkeit stets, bei Berücksichtigung derselben wenigstens dann, wenn es sich um das *Einelektronenproblem* handelt, auf die Gestalt bringen: quadratische

Annalen der Physik, vol. 385, Issue 13, p437, 1926.

# The Schrödinger equation (4)

For a one-dimensional problem and with $V = 0$ :

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} = E\phi$$

or,

$$\frac{d^2\phi}{dx^2} + \frac{2mE}{\hbar^2}\phi = 0$$

we pose $k^2 = 2mE/\hbar^2$ and the general solution writes :

$$\Psi(x,t) = \phi(x)T(t) = \left\{ \begin{array}{c} \sin kx \\ \cos kx \end{array} \right\} e^{-iEt/\hbar}$$

# The Schrödinger equation - Example (1)

Example : Particle in a box ($V = 0$ on [0,L], $\Psi = 0$ at $x = 0, L\ \forall t$)

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- $\Psi(x=L,t) = 0$ requires

$$k = n\pi/L$$

which leads to

$$E_n = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2}$$

$\Rightarrow$ In quantum mechanics, the energy of a particle traped between 0 and L can have only a discrete set of values called eigenvalues : the energy is quantised.

# The Schrödinger equation - Example (2)

The basis functions are then :

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The general solution is then a linear combination these :

$$\Psi(x,t) = \sum_{n=1}^{\infty} b_n \sin\frac{n\pi x}{L}e^{-iE_nt/\hbar}$$

# Numerical benchmarking

The heat transport equation writes :

$$\rho c_p \left( \frac{\partial T}{\partial t} + \underbrace{\mathbf{v} \cdot \boldsymbol{\nabla} T}_{adv.} \right) = \underbrace{\boldsymbol{\nabla} \cdot (k \boldsymbol{\nabla} T)}_{diff.} + \underbrace{H}_{prod.}$$

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This translates as follows in my geodynamics numerical code :

```
Ka3D=matmul(NvectTstar3D,matmul(vel3D,Bmat3D))*rho*hcapa*JxW

Kc3D=matmul(BmatT3D,Bmat3D)*hcond*JxW

KK3D=(Ka3D+Kc3D)

M3D=matmul(NvectT3D,Nvect3D)*rho*hcapa*JxW

F3D=N3D(:,iq)*JxW*hprod

Ael=Ael+(M3D+KK3D*alphaT*dt)
Bel=Bel+matmul(M3D-KK3D*(1.d0-alphaT)*dt,temp(1:8))+F3D*dt
```

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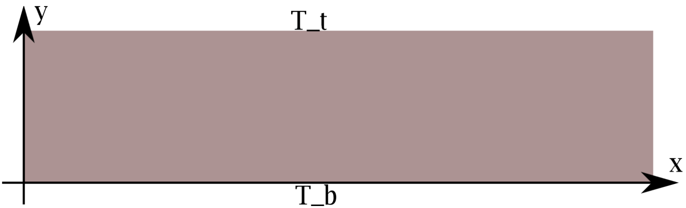
- wall diffusion (1D)
- cone diffusion (2D)

# 1D diffusion benchmark (1)




- system with initial uniform temperature of 0 heated from below.

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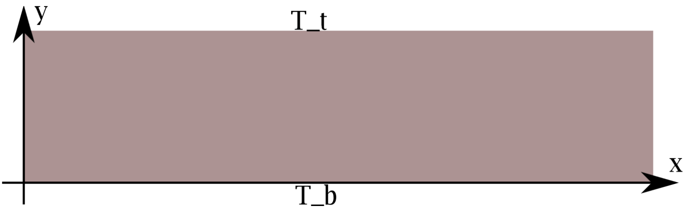


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- temperature at the top of the system is set to 0.
- imposed temperature at the bottom is 1.

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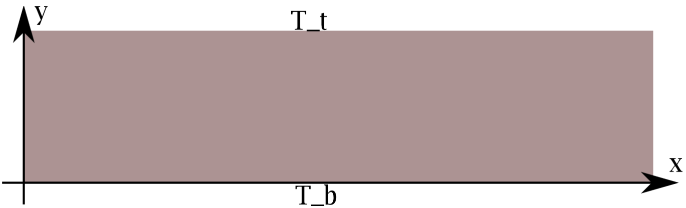


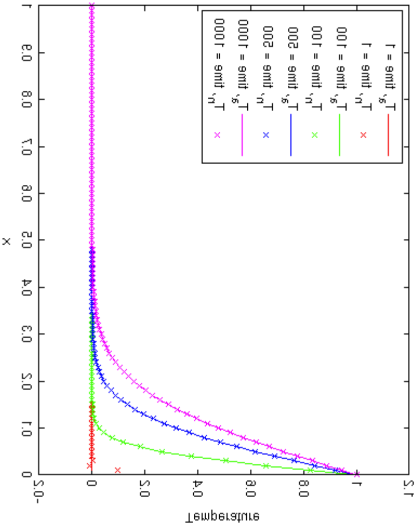

- system with initial uniform temperature of 0 heated from below.
- temperature at the top of the system is set to 0.
- imposed temperature at the bottom is 1.
- The analytical solution, in a $T - y$-coordinate system, is,

$$T_{analytical} = erfc(\frac{y}{2\sqrt{\kappa t}})(T_b - T_t) + T_t$$

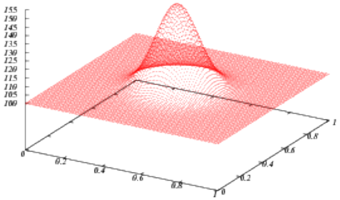
where $y$ is the distance from the bottom to the top of the system, $T_b$ is the temperature imposed at the bottom and $T_t$ is the temperature at the top.

# 1D diffusion benchmark (2)

Computed temperature profiles at successive timesteps :



# 2D diffusion benchmark (1)

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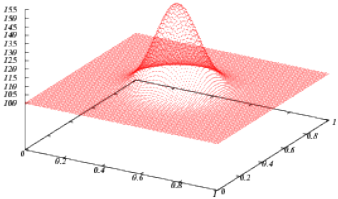

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- The initial temperature profile is placed in the centre of the domain $(x_c, y_c)$, and we observe how it diffuses in time. (initial Gaussian temperature profile).

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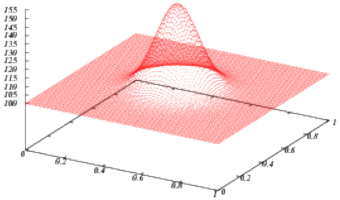

- domain is unit square $[0, 1] \times [0, 1]$
- The initial temperature profile is placed in the centre of the domain $(x_c, y_c)$, and we observe how it diffuses in time. (initial Gaussian temperature profile).
- The diffusion observed should be described by the analytical solution given by the Gaussian function

$$T(x, y, t) = \frac{t_0}{t} \exp\left(-\frac{(x - x_c)^2 + (y - y_c)^2}{4\kappa t}\right)$$

# 2D diffusion benchmark (2)

The temperature field gradually decreases in height and broadens in width.