

Nome: Matheus Muviz

Lista Introdução à Modelagem Computacional

1) a) $\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y} \right)$

com $f(x, y) = \sin(x) \cos(y)$

$$\frac{\partial f}{\partial x} = \cos(x) \cos(y)$$

$$\frac{\partial f}{\partial y} = -\sin(x) \sin(y)$$

$$\nabla f = (\cos(x) \cos(y), -\sin(x) \sin(y))$$

b) $\Delta f = \nabla \cdot (\nabla f) = \nabla^2 f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$

$$\Delta f = \frac{\partial}{\partial x} (\cos(x) \cos(y)) + \frac{\partial}{\partial y} (-\sin(x) \sin(y))$$

$$\Delta f = -\sin(x) \cos(y) - \sin(x) \cos(y) = -2 \sin(x) \cos(y)$$

c) Gráfico junto ao trabalho do solven.

a) $f(x, y) = 3x^2 + 5y^2$

$$\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y} \right) \rightarrow \nabla f = (6x, 10y)$$

b) $\Delta f = \frac{\partial}{\partial x} (6x) + \frac{\partial}{\partial y} (10y) \rightarrow \Delta f = 16$

c) Gráfico junto ao trabalho do solven.

2) $f(x, y, z) = \cos(xy) e^{2z}$

a) $\nabla f = (\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z})$

$$\frac{\partial f}{\partial x} = -y \sin(xy) e^{2z}$$

$$\frac{\partial f}{\partial y} = -x \sin(xy) e^{2z}$$

$$\frac{\partial f}{\partial z} = 2 \cos(xy) e^{2z}$$

Logo $\nabla f = (-y \sin(xy) e^{2z}, -x \sin(xy) e^{2z}, 2 \cos(xy) e^{2z})$

b) $\Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$

$$\frac{\partial^2 f}{\partial x^2} = -y^2 \cos(xy) e^{2z}$$

$$\frac{\partial^2 f}{\partial y^2} = -x^2 \cos(xy) e^{2z}$$

$$\frac{\partial^2 f}{\partial z^2} = 4 \cos(xy) e^{2z}$$

Logo $\Delta f = e^{2z} \cos(xy) (4 - x^2 - y^2)$

c) $\Delta(f \cdot f) = \Delta(f \cdot f) = \frac{\partial^2 (f \cdot f)}{\partial x^2} + \frac{\partial^2 (f \cdot f)}{\partial y^2}$

$$\frac{\partial^2 (f \cdot f)}{\partial x^2} = \frac{\partial}{\partial x} \left(\frac{\partial f}{\partial x} f + \frac{\partial f}{\partial x} f \right) = 2 \frac{\partial f}{\partial x} \cdot \frac{\partial f}{\partial x}$$

$$\frac{\partial^2 (f \cdot f)}{\partial y^2} = 2 \frac{\partial f}{\partial y} \cdot \frac{\partial f}{\partial y}$$

$$\Delta(f)^2 = 2 \cdot \frac{2}{2x} \cdot \left(f \cdot \frac{2f}{2x} \right) + 2 \frac{2}{2y} \left(f \cdot \frac{2f}{2y} \right) \quad \Delta(f)^2 = 2 \left[\frac{2f}{2x} \cdot \frac{2f}{2x} + f \frac{2^2 f}{2x^2} \right] + 2 \left[\frac{2f}{2y} \cdot \frac{2f}{2y} + f \frac{2^2 f}{2y^2} \right]$$

$$\Delta(f)^2 = 2 \left(\frac{2f}{2x} \right)^2 + 2f \frac{2^2 f}{2x^2} + 2 \left(\frac{2f}{2y} \right)^2 + 2f \frac{2^2 f}{2y^2} \quad \Delta(f)^2 = 2 \cdot \nabla f \cdot \nabla f + 2f \cdot \Delta f$$

$$\nabla f \cdot \nabla f = \left(\frac{2f}{2x} \right)^2 + \left(\frac{2f}{2y} \right)^2 + \left(\frac{2f}{2z} \right)^2 \quad \nabla f \cdot \nabla f = y^2 \sin^2(xy) e^{4z} + x^2 \sin^2(xy) e^{4z} + 4 \cos^2(xy) e^{4z}$$

$$f \cdot \Delta f = e^{4z} \cos^2(xy) (4 - x^2 - y^2)$$

Logo:

$$\Delta(f)^2 = 2y^2 \sin^2(xy) e^{4z} + 2x^2 \sin^2(xy) e^{4z} + 8 \cos^2(xy) e^{4z} + 8 \cos^2(xy) e^{4z} - 2x^2 \cos^2(xy) e^{4z} - 2y^2 \cos^2(xy) e^{4z}$$

$$\Delta(f)^2 = 16 \cos^2(xy) e^{4z} + 2y^2 e^{4z} (\sin^2(xy) - \cos^2(xy)) + 2x^2 e^{4z} (\sin^2(xy) - \cos^2(xy)) \quad \left| \sin^2(xy) = 1 - \cos^2(xy) \right|$$

$$\Delta(f)^2 = 16 \cos^2(xy) e^{4z} + 2y^2 e^{4z} (1 - 2\cos^2(xy)) + 2x^2 e^{4z} (1 - \cos^2(xy))$$

$$\Delta(f)^2 = (16 - 4x^2 - 4y^2) e^{4z} \cos^2(xy) + (2x^2 + 2y^2) e^{4z}$$

$$3) a) \frac{\partial P}{\partial t} = \frac{1}{4\pi} \frac{2}{2t} \left(\frac{1}{t} e^{2t} \cdot e^{-\frac{x^2+y^2}{4t}} \right) \rightarrow \frac{\partial P}{\partial t} = \frac{1}{4\pi} \left[\frac{\partial}{\partial t} \left(\frac{1}{t} \right) \cdot e^{-\frac{x^2+y^2}{4t}} + \frac{1}{t} \frac{\partial}{\partial t} \left(e^{-\frac{x^2+y^2}{4t}} \right) \right]$$

$$\frac{\partial P}{\partial t} = \frac{1}{4\pi} \left[\left[\frac{\partial}{\partial t} \left(\frac{1}{t} \right) \cdot e^{2t} + \frac{1}{t} \frac{\partial}{\partial t} (e^{2t}) \right] \cdot e^{-\frac{x^2+y^2}{4t}} + \frac{1}{t} \cdot e^{-\frac{x^2+y^2}{4t}} \cdot \frac{\partial}{\partial t} \left(-\frac{x^2+y^2}{4t} \right) \right]$$

$$\frac{\partial P}{\partial t} = \frac{1}{4\pi} \left\{ \left[\frac{-e^{2t}}{t^2} + \frac{2e^{2t}}{t} \right] e^{-\frac{x^2+y^2}{4t}} + \frac{e^{2t}}{t} \cdot e^{-\frac{x^2+y^2}{4t}} \cdot \frac{x^2+y^2}{4t^2} \right\}$$

$$\frac{\partial P}{\partial t} = \frac{-e^{2t}}{4\pi t^2} e^{-\frac{x^2+y^2}{4t}} + \frac{e^{2t}}{2\pi t} e^{-\frac{x^2+y^2}{4t}} + \frac{e^{2t}}{4\pi t} e^{-\frac{x^2+y^2}{4t}} \cdot \left(\frac{x^2+y^2}{4t} \right)$$

$$\frac{\partial P}{\partial t} = \frac{-x}{8\pi t^2} e^{2t} e^{-\frac{x^2+y^2}{4t}} \rightarrow \frac{\partial^2 P}{\partial x^2} = \frac{-e^{2t}}{8\pi t^2} \frac{\partial}{\partial x} \left(x \cdot e^{-\frac{x^2+y^2}{4t}} \right) \rightarrow \frac{\partial^2 P}{\partial x^2} = \frac{-e^{2t}}{8\pi t^2} \left(e^{-\frac{x^2+y^2}{4t}} - \frac{x^2}{2t} e^{-\frac{x^2+y^2}{4t}} \right) \rightarrow$$

$$\frac{\partial^2 P}{\partial x^2} = \frac{-e^{2t}}{8\pi t^2} e^{-\frac{x^2+y^2}{4t}} + \frac{x^2 e^{2t}}{16\pi t^3} e^{-\frac{x^2+y^2}{4t}}$$

$$\frac{\partial^2 P}{\partial y^2} = \frac{-e^{2t}}{8\pi t^2} e^{-\frac{x^2+y^2}{4t}} + \frac{y^2 e^{2t}}{16\pi t^3} e^{-\frac{x^2+y^2}{4t}}$$

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + 2P = \frac{-e^{2t}}{4\pi t^2} e^{-\frac{x^2+y^2}{4t}} + \frac{e^{2t}}{16\pi t^3} e^{-\frac{x^2+y^2}{4t}} (x^2+y^2) + \frac{e^{2t}}{2\pi t} e^{-\frac{x^2+y^2}{4t}} = \frac{\partial P}{\partial t}$$

b) junto ao trabalho ao solver

4) $r = \sqrt{x^2 + y^2}$ e $\theta = \tan^{-1}(y/x)$

$$\frac{\partial r}{\partial x} = \frac{2x}{2\sqrt{x^2 + y^2}} = \frac{x}{r} = \cos \theta \quad \frac{\partial \theta}{\partial x} = \frac{-y}{x^2 + y^2} = -\frac{\sin \theta}{r}$$

$P = P(r, \theta)$

$$\frac{\partial r}{\partial y} = \frac{2y}{2\sqrt{x^2 + y^2}} = \frac{y}{r} = \sin \theta \quad \frac{\partial \theta}{\partial y} = \frac{x}{x^2 + y^2} = \frac{\cos \theta}{r}$$

$$\frac{\partial P}{\partial x} = \frac{\partial P}{\partial r} \frac{\partial r}{\partial x} + \frac{\partial P}{\partial \theta} \frac{\partial \theta}{\partial x} \rightarrow \frac{\partial P}{\partial x} = \cos \theta \frac{\partial P}{\partial r} - \frac{\sin \theta}{r} \frac{\partial P}{\partial \theta}$$

$$\frac{\partial P}{\partial y} = \frac{\partial P}{\partial r} \frac{\partial r}{\partial y} + \frac{\partial P}{\partial \theta} \frac{\partial \theta}{\partial y} \rightarrow \frac{\partial P}{\partial y} = \sin \theta \frac{\partial P}{\partial r} + \frac{\cos \theta}{r} \frac{\partial P}{\partial \theta}$$

$$\frac{\partial^2 P}{\partial x^2} = \frac{\partial}{\partial x} \left(\cos \theta \frac{\partial P}{\partial r} - \frac{\sin \theta}{r} \frac{\partial P}{\partial \theta} \right) = \frac{\partial}{\partial x} \left(\cos \theta \right) \frac{\partial P}{\partial r} + \cos \theta \left(\frac{\partial^2 P}{\partial r^2} \frac{\partial r}{\partial x} + \frac{\partial^2 P}{\partial r \partial \theta} \frac{\partial \theta}{\partial x} \right) - \frac{\partial}{\partial x} \left(\frac{\sin \theta}{r} \right) \frac{\partial P}{\partial \theta} - \frac{\sin \theta}{r} \left(\frac{\partial^2 P}{\partial r \partial \theta} \frac{\partial r}{\partial x} + \frac{\partial^2 P}{\partial \theta^2} \frac{\partial \theta}{\partial x} \right)$$

$$\frac{\partial^2 P}{\partial x^2} = -\sin \theta \frac{\partial \theta}{\partial x} \frac{\partial P}{\partial r} + \cos \theta \frac{\partial^2 P}{\partial r^2} \frac{\partial r}{\partial x} + \cos \theta \frac{\partial^2 P}{\partial r \partial \theta} \frac{\partial \theta}{\partial x} - \left(\frac{\partial \sin \theta}{\partial x} \frac{1}{r} - \frac{\sin \theta}{r^2} \frac{\partial r}{\partial x} \right) \frac{\partial P}{\partial \theta} - \frac{\sin \theta}{r} \frac{\partial^2 P}{\partial r \partial \theta} \frac{\partial r}{\partial x} - \frac{\sin \theta}{r} \frac{\partial^2 P}{\partial \theta^2} \frac{\partial \theta}{\partial x}$$

$$\frac{\partial^2 P}{\partial x^2} = \frac{\sin^2 \theta}{r} \frac{\partial P}{\partial r} + \cos^2 \theta \frac{\partial^2 P}{\partial r^2} + \cos^2 \theta \frac{\partial^2 P}{\partial r \partial \theta} - \frac{\sin \theta \cos \theta}{r} \frac{\partial^2 P}{\partial \theta^2} - \frac{1}{r^2} \frac{\partial P}{\partial \theta} \left(\cos \theta r \frac{\partial \theta}{\partial x} - \sin \theta \cos \theta \right) - \frac{\sin \theta \cos \theta}{r} \frac{\partial^2 P}{\partial r \partial \theta} + \frac{\sin^2 \theta}{r^2} \frac{\partial^2 P}{\partial \theta^2}$$

$$\frac{\partial^2 P}{\partial x^2} = \frac{\sin^2 \theta}{r} \frac{\partial P}{\partial r} + \cos^2 \theta \frac{\partial^2 P}{\partial r^2} - 2 \frac{\sin \theta \cos \theta}{r} \frac{\partial^2 P}{\partial r \partial \theta} + \frac{\sin^2 \theta}{r^2} \frac{\partial^2 P}{\partial \theta^2} + \frac{2 \sin \theta \cos \theta}{r^2} \frac{\partial P}{\partial \theta} \quad \textcircled{I}$$

$$\frac{\partial^2 P}{\partial y^2} = \frac{2 \sin \theta}{2y} \frac{\partial P}{\partial r} + \sin \theta \left(\frac{\partial^2 P}{\partial r^2} \frac{\partial r}{\partial y} + \frac{\partial^2 P}{\partial r \partial \theta} \frac{\partial \theta}{\partial y} \right) + \frac{\partial}{\partial y} \left(\frac{\cos \theta}{r} \right) \frac{\partial P}{\partial \theta} + \frac{\cos \theta}{r} \left(\frac{\partial^2 P}{\partial r \partial \theta} \frac{\partial r}{\partial y} + \frac{\partial^2 P}{\partial \theta^2} \frac{\partial \theta}{\partial y} \right)$$

$$\frac{\partial^2 P}{\partial y^2} = \cos \theta \frac{\partial \theta}{\partial y} \frac{\partial P}{\partial r} + \sin \theta \left(\sin \theta \frac{\partial^2 P}{\partial r^2} + \cos \theta \frac{\partial^2 P}{\partial r \partial \theta} \right) + \left(\frac{\partial \cos \theta}{\partial y} \frac{1}{r} - \frac{\cos \theta}{r^2} \frac{\partial r}{\partial y} \right) \frac{\partial P}{\partial \theta} + \frac{\cos \theta}{r} \left(\sin \theta \frac{\partial^2 P}{\partial r \partial \theta} + \cos \theta \frac{\partial^2 P}{\partial \theta^2} \right)$$

$$\frac{\partial^2 P}{\partial y^2} = \frac{\cos^2 \theta}{r} \frac{\partial P}{\partial r} + \sin^2 \theta \frac{\partial^2 P}{\partial r^2} + \sin \theta \cos \theta \frac{\partial^2 P}{\partial r \partial \theta} + \sin \theta \cos \theta \frac{\partial^2 P}{\partial r \partial \theta} + \frac{\cos^2 \theta}{r^2} \frac{\partial^2 P}{\partial \theta^2} + \frac{1}{r^2} \frac{\partial P}{\partial \theta} \left(-\sin \theta \frac{\partial \theta}{\partial y} r - \cos \theta \frac{\partial r}{\partial y} \right)$$

$$\frac{\partial^2 P}{\partial y^2} = \frac{\cos^2 \theta}{r} \frac{\partial P}{\partial r} + \sin^2 \theta \frac{\partial^2 P}{\partial r^2} + 2 \frac{\sin \theta \cos \theta}{r} \frac{\partial^2 P}{\partial r \partial \theta} + \frac{\cos^2 \theta}{r^2} \frac{\partial^2 P}{\partial \theta^2} - 2 \frac{\sin \theta \cos \theta}{r^2} \frac{\partial P}{\partial \theta} \quad \textcircled{II}$$

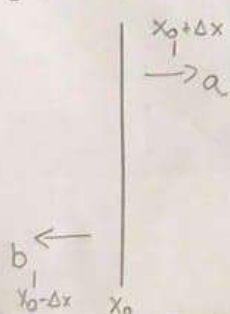
$\textcircled{I} + \textcircled{II}$:

$$\Delta P = \frac{\partial^2 P}{\partial r^2} + \frac{1}{r} \frac{\partial P}{\partial r} + \frac{1}{r^2} \frac{\partial^2 P}{\partial \theta^2}$$

Simetria Radial

$$\frac{\partial^2 P}{\partial t^2} = \frac{\partial}{\partial t} \left(\frac{\partial^2 P}{\partial r^2} + \frac{1}{r} \frac{\partial P}{\partial r} \right)$$

5)

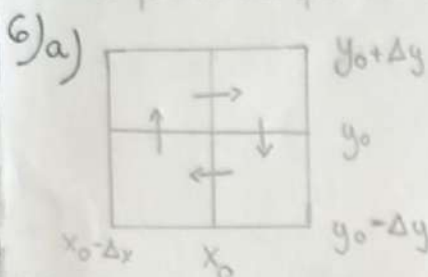


$$J\Delta t = (-a P_{(x_0+\Delta x, t)} + b P_{(x_0-\Delta x, t)}) \Delta x \quad \left| \begin{array}{l} P_{(x_0+\Delta x, t)} = P_{(x_0, t)} + \frac{\partial P_{(x_0, t)}}{\partial x} \Delta x \\ P_{(x_0-\Delta x, t)} = P_{(x_0, t)} - \frac{\partial P_{(x_0, t)}}{\partial x} \Delta x \end{array} \right.$$

$$J\Delta t = (-a P - a \Delta x \frac{\partial P}{\partial x} + b P - b \Delta x \frac{\partial P}{\partial x}) \Delta x \quad \left| \begin{array}{l} J = -(a-b) \Delta x P - (a+b) \Delta x^2 \frac{\partial P}{\partial x} \end{array} \right.$$

$$\frac{\partial P}{\partial t} = -\frac{\partial J}{\partial x} \rightarrow \frac{\partial P}{\partial t} = \frac{-(a-b) \Delta x}{\Delta t} \frac{\partial P}{\partial x} + \frac{(a+b) \Delta x^2}{\Delta t} \frac{\partial^2 P}{\partial x^2} \quad \left[\underbrace{\frac{\partial P}{\partial t} - \frac{(a-b) \Delta x}{\Delta t} \frac{\partial P}{\partial x}}_V = \underbrace{\frac{(a+b) \Delta x^2}{\Delta t} \frac{\partial^2 P}{\partial x^2}}_D \right]$$

Temos problemas quando $a=1$ e $b=0$ ou $a=0$ e $b=1$ (temos em que não existe difusão).



Vamos supor a probabilidade de movimento em cada sentido como $\frac{1}{2}$.

$$J_x = \frac{1}{2} (-P_{(x_0+\Delta x, t)} + P_{(x_0-\Delta x, t)}) \frac{\Delta x}{\Delta t} \quad \begin{array}{l} P_{(x_0+\Delta x, t)} = P + \frac{\partial P}{\partial x} \Delta x \\ P_{(x_0-\Delta x, t)} = P - \frac{\partial P}{\partial x} \Delta x \end{array}$$

$$J_x = -\left(\frac{\Delta x^2}{2\Delta t}\right) \frac{\partial^2 P}{\partial x^2}$$

$$J_y = \frac{1}{2} (-P_{(y_0+\Delta y, t)} + P_{(y_0-\Delta y, t)}) \frac{\Delta y}{\Delta t} \quad \begin{array}{l} P_{(y_0+\Delta y, t)} = P + \frac{\partial P}{\partial y} \Delta y \\ P_{(y_0-\Delta y, t)} = P - \frac{\partial P}{\partial y} \Delta y \end{array}$$

$$J_y = -\left(\frac{\Delta y^2}{2\Delta t}\right) \frac{\partial^2 P}{\partial y^2}$$

Logo:

$$\frac{\partial P}{\partial t} = -\nabla \cdot \vec{J}$$

$$\frac{\partial P}{\partial t} = -\left(\frac{2J_x}{2x} + \frac{2J_y}{2y}\right)$$

$$\frac{\partial P}{\partial t} = +\left[\underbrace{\left(\frac{\Delta x^2}{2\Delta t}\right)}_{D_x} \frac{\partial^2 P}{\partial x^2} + \underbrace{\left(\frac{\Delta y^2}{2\Delta t}\right)}_{D_y} \frac{\partial^2 P}{\partial y^2}\right]$$

Supondo um meio isotrópico $\Delta x = \Delta y \rightarrow D_x = D_y = D$

$$\frac{\partial P}{\partial t} = D \left(\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} \right)$$

Nome: Matheus Muniz

Lista Introdução a Modelagem Computacional

$$6) b) \begin{cases} X = ax + by & x = b \\ Y = -bx + ay & x = a \end{cases} \rightarrow \begin{cases} bX = abx + b^2y \\ aY = -abx + a^2y \end{cases} \rightarrow (a^2 + b^2)y = bX + aY \rightarrow y = \frac{bX + aY}{a^2 + b^2}$$

$$\begin{cases} X = ax + by & x = a \\ Y = -bx + ay & x = b \end{cases} \rightarrow \begin{cases} aX = a^2x + aby \\ -bY = -b^2x + aby \end{cases} \rightarrow (a^2 + b^2)x = aX - bY \rightarrow x = \frac{aX - bY}{a^2 + b^2}$$

Transformações inversas $\begin{cases} x = \frac{aX - bY}{a^2 + b^2} \rightarrow x = x(x, y) \\ y = \frac{bX + aY}{a^2 + b^2} \rightarrow y = y(x, y) \end{cases}$

$$\Delta_{xy} u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \text{ mas } u = u(x, y) = u(x(x, y), y(x, y))$$

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial x} \cdot \frac{\partial x}{\partial X} + \frac{\partial u}{\partial y} \cdot \frac{\partial y}{\partial X} = \frac{\partial u}{\partial x} \cdot a + \frac{\partial u}{\partial y} \cdot b$$

$$\frac{\partial^2 u}{\partial x^2} = \left(\frac{\partial^2 u}{\partial x^2} \frac{\partial x}{\partial X} + \frac{\partial^2 u}{\partial y \partial x} \frac{\partial y}{\partial X} \right) a + \left(\frac{\partial^2 u}{\partial x \partial y} \frac{\partial x}{\partial X} + \frac{\partial^2 u}{\partial y^2} \frac{\partial y}{\partial X} \right) b$$

$$\frac{\partial^2 u}{\partial x^2} = \left(\frac{\partial^2 u}{\partial x^2} \cdot a + \frac{\partial^2 u}{\partial y \partial x} \cdot b \right) a + \left(\frac{\partial^2 u}{\partial x \partial y} \cdot a + \frac{\partial^2 u}{\partial y^2} \cdot b \right) b$$

$$\frac{\partial^2 u}{\partial x^2} = a^2 \frac{\partial^2 u}{\partial x^2} + b^2 \frac{\partial^2 u}{\partial y^2} + ab \frac{\partial^2 u}{\partial y \partial x} + ab \frac{\partial^2 u}{\partial x \partial y} \quad (I)$$

$$\frac{\partial u}{\partial Y} = \frac{\partial u}{\partial x} \cdot \frac{\partial x}{\partial Y} + \frac{\partial u}{\partial y} \cdot \frac{\partial y}{\partial Y} = -b \frac{\partial u}{\partial x} + a \frac{\partial u}{\partial y}$$

$$\frac{\partial^2 u}{\partial Y^2} = -b \left(\frac{\partial^2 u}{\partial x^2} \frac{\partial x}{\partial Y} + \frac{\partial^2 u}{\partial y \partial x} \frac{\partial y}{\partial Y} \right) + a \left(\frac{\partial^2 u}{\partial x \partial y} \frac{\partial x}{\partial Y} + \frac{\partial^2 u}{\partial y^2} \frac{\partial y}{\partial Y} \right)$$

$$\frac{\partial^2 u}{\partial Y^2} = -b \left(-b \frac{\partial^2 u}{\partial x^2} + a \frac{\partial^2 u}{\partial y \partial x} \right) + a \left(-b \frac{\partial^2 u}{\partial x \partial y} + a \frac{\partial^2 u}{\partial y^2} \right)$$

$$\frac{\partial^2 u}{\partial Y^2} = b^2 \frac{\partial^2 u}{\partial x^2} + a^2 \frac{\partial^2 u}{\partial y^2} - ab \frac{\partial^2 u}{\partial y \partial x} - ab \frac{\partial^2 u}{\partial x \partial y} \quad (II)$$

$$(I) + (II): \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = (a^2 + b^2) \frac{\partial^2 u}{\partial x^2} + (a^2 + b^2) \frac{\partial^2 u}{\partial y^2}$$

$$\Delta_{xy} u = \Delta_{xy} u$$

c) Como foi feito em a) de forma geral, vê-se que devemos assumir que a difusividade é igual em cada direção. Isso vem com a suposição de que $\Delta x = \Delta y$, ou seja, a população percorre a mesma distância no mesmo tempo em cada direção.

7) Considere o domínio Ω com borda $\partial\Omega$ e normal exterior \vec{n} . O termo de reação é $f(t, x, P)$.



Supondo que o movimento ocorre em uma direção preferencial \vec{Y} e \mathbb{R}^n .

Temos:

$$\underbrace{\frac{d}{dt} \left(\int_{\Omega} P(t, x) dx \right)}_{\text{Variação temporal dentro de } \Omega} = \underbrace{\int_{\Omega} f(t, x, P) dx}_{\text{Quantidade gerada ou criada em } \Omega} - \underbrace{\int_{\partial\Omega} \vec{J}(t, x) \cdot \vec{n}(x) ds}_{\text{Quantidade que entra ou sai de } \Omega}$$

O fluxo ocorre de acordo com a direção preferencial a uma velocidade V , daí:

$$\vec{J} = \overset{\text{Advecção}}{V P(t, x) \vec{Y}} - \underset{\text{Difusão}}{D \nabla P}$$

$$\frac{d}{dt} \left(\int_{\Omega} P dx \right) = - \int_{\partial\Omega} (V P \vec{Y} - D \nabla P) \cdot \vec{n} ds + \int_{\Omega} f dx$$

De acordo com o Teorema de Gauss:

$$\int_{\partial\Omega} (V P \vec{Y} - D \nabla P) \cdot \vec{n} ds = \int_{\Omega} \nabla \cdot (V P \vec{Y} - D \nabla P) dx$$

Assumindo que Ω está bem definido, pode-se eliminar com $\frac{d}{dt}$ para dentro da integral:

$$\int_{\Omega} \frac{\partial P}{\partial t} dx = - \int_{\Omega} \nabla \cdot (V P \vec{Y} - D \nabla P) dx + \int_{\Omega} f dx$$

Como Ω é geral, temos:

$$\frac{\partial P}{\partial t} = - \nabla \cdot (V P \vec{Y}) + D \underbrace{\nabla \cdot (\nabla P)}_{\Delta P} + f$$

Supondo que V é constante:

$$\nabla \cdot (V P \vec{Y}) = V \nabla \cdot (P \vec{Y}) \rightarrow V \vec{\nabla} \cdot (P \vec{Y}) = V \left(\frac{\partial P}{\partial x} Y_1 + \frac{\partial P}{\partial y} Y_2 + \dots + \frac{\partial P}{\partial w^n} Y_n \right) \vec{Y}$$

$\nabla P \vec{Y} \rightsquigarrow$ Gradiente

$$\frac{\partial P}{\partial t} = -V \nabla P \vec{Y} + D \Delta P + f \rightarrow \boxed{\frac{\partial P}{\partial t} + V \nabla P \cdot \vec{Y} = D \Delta P + f} \rightsquigarrow \text{Equação Advecção, Difusão, reação}$$

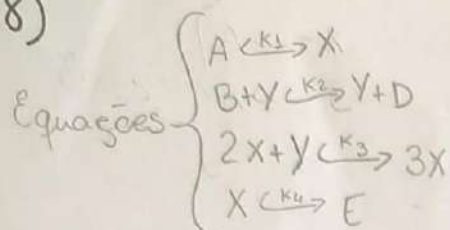
No caso 1D $\rightarrow \vec{Y} = \hat{x}$.

$$\frac{\partial P}{\partial t} + V \frac{\partial P}{\partial x} = D \frac{\partial^2 P}{\partial x^2} + f$$

Nome: Matheus Muniz

Lista Introdução à Modelagem Computacional

8)



Suponha que A e B são "alimentados" de modo que sua concentração constante. Escreva em sistemas de equações de reação-difusão para X e Y. Considere d_x e d_y os coeficientes de difusão de X e Y, respectivamente.

$$\frac{\partial X}{\partial t} = d_x \Delta X + K_1 A + K_3 X^2 Y - K_4 X$$

$$\frac{\partial Y}{\partial t} = d_y \Delta Y - K_2 B Y + K_2 B Y - K_3 X^2 Y = d_y \Delta Y - K_3 X^2 Y$$

9)

$C(0, x) = 0 \rightarrow$ inicialmente, apenas água pura.

$$C(t, 0) = C_3$$

$$C(t, L) = C_2$$

b) Queremos uma função linear $f(x) = ax + b$ tal que $f(0) = C_3$ e $f(L) = 0$.

$$f(0) = a \cdot 0 + b = C_3 \rightarrow b = C_3$$

$$f(L) = a \cdot L + C_3 = 0 \rightarrow a = -\frac{C_3}{L}$$

$$\text{então, } f(x) = -\frac{C_3}{L}x + C_3$$

$$C(0, x) = -\frac{C_3}{L}x + C_3$$

$$\frac{\partial C}{\partial t}(t, 0) = 0; \text{ tubo selado em } x=0.$$

$$C(t, L) = 0; \text{ concentração constante em } x=L.$$

Matheus Muniz Damasco
Parte 1 - Lista de Exercícios

1 - c) Os códigos usados no Python para gerar os gráficos das duas superfícies são exibidos nas figuras a seguir:

Gráfico 1:

```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D

x = np.linspace(-2, 2, 40)
y = x
x, y = np.meshgrid(x, y)
z = np.sin(x) * np.cos(y)

fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
surf = ax.plot_surface(x, y, z, cmap='viridis')

ax.set_xlabel('x')
ax.set_ylabel('y')
ax.set_zlabel('z')
ax.set_title('sin(x)cos(y)')

plt.show()
```

Gráfico 2:

```
x = np.linspace(-2, 2, 40)
y = x[:, np.newaxis]
z = 3 * x**2 + 5 * y**2

fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
surf = ax.plot_surface(x, y, z, cmap='viridis')

ax.set_xlabel('x')
ax.set_ylabel('y')
ax.set_zlabel('z')
ax.set_title('3x^2 + 5y^2')

plt.show()
```

Os resultados foram as superfícies no espaço cartesiano das figuras abaixo:

Gráfico 1:

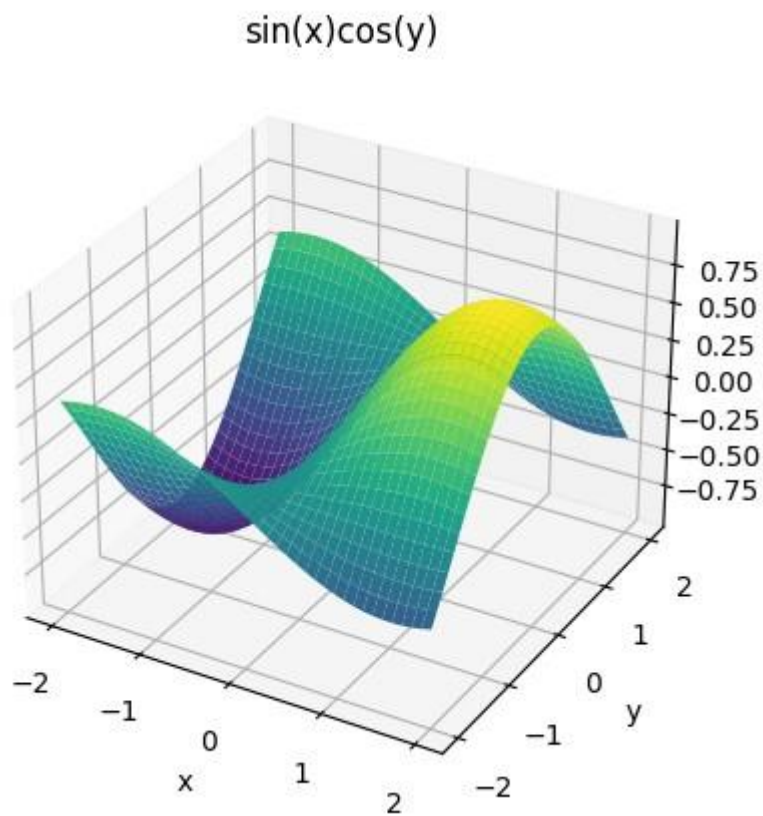
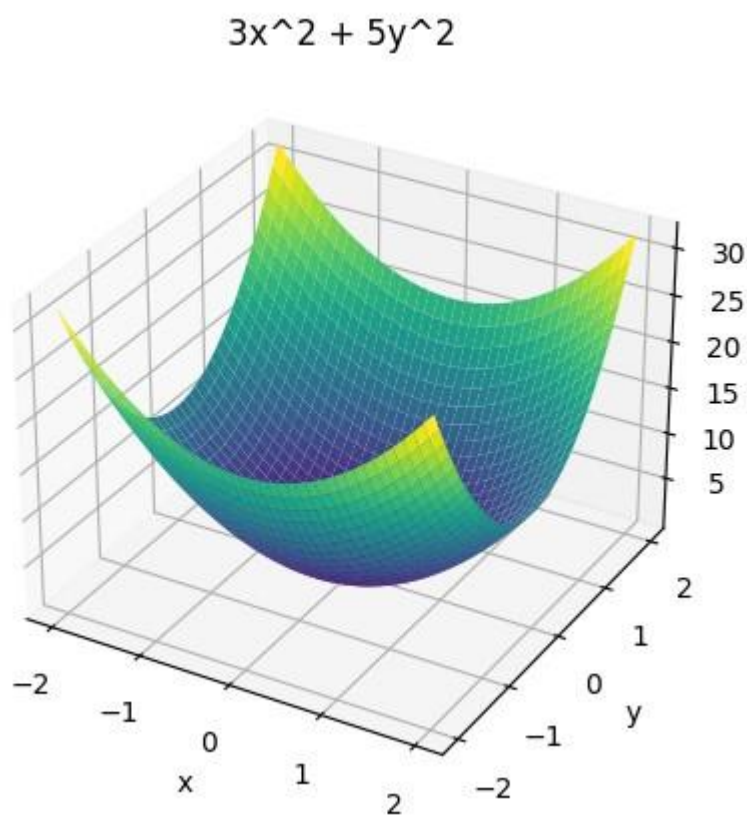


Gráfico 2:



Como esperado, a primeira superfície é ondulada, já a segunda é um parabolóide elíptico.

Gráfico 3:

```
x = np.linspace(-8, 8, 100)
y = np.linspace(-8, 8, 100)
X, Y = np.meshgrid(x, y)
Z = np.sin(X) * np.cos(Y)

plt.contour(X, Y, Z)
plt.title("Curvas de Nível para sin(x)cos(y)")
plt.xlabel("x")
plt.ylabel("y")
plt.show()
```

Gráfico 4:

```
x = np.linspace(-8, 8, 100)
y = np.linspace(-8, 8, 100)
X, Y = np.meshgrid(x, y)
Z = 3 * X**2 + 5 * Y**2

plt.contour(X, Y, Z)
plt.title("Curvas de Nível para 3x^2 + 5y^2")
plt.xlabel("x")
plt.ylabel("y")
plt.show()
```

O produto das compilações desses códigos foram as projeções das curvas de nível para cada função no plano xOy, as figuras a seguir mostram os resultados:

Gráfico 3:

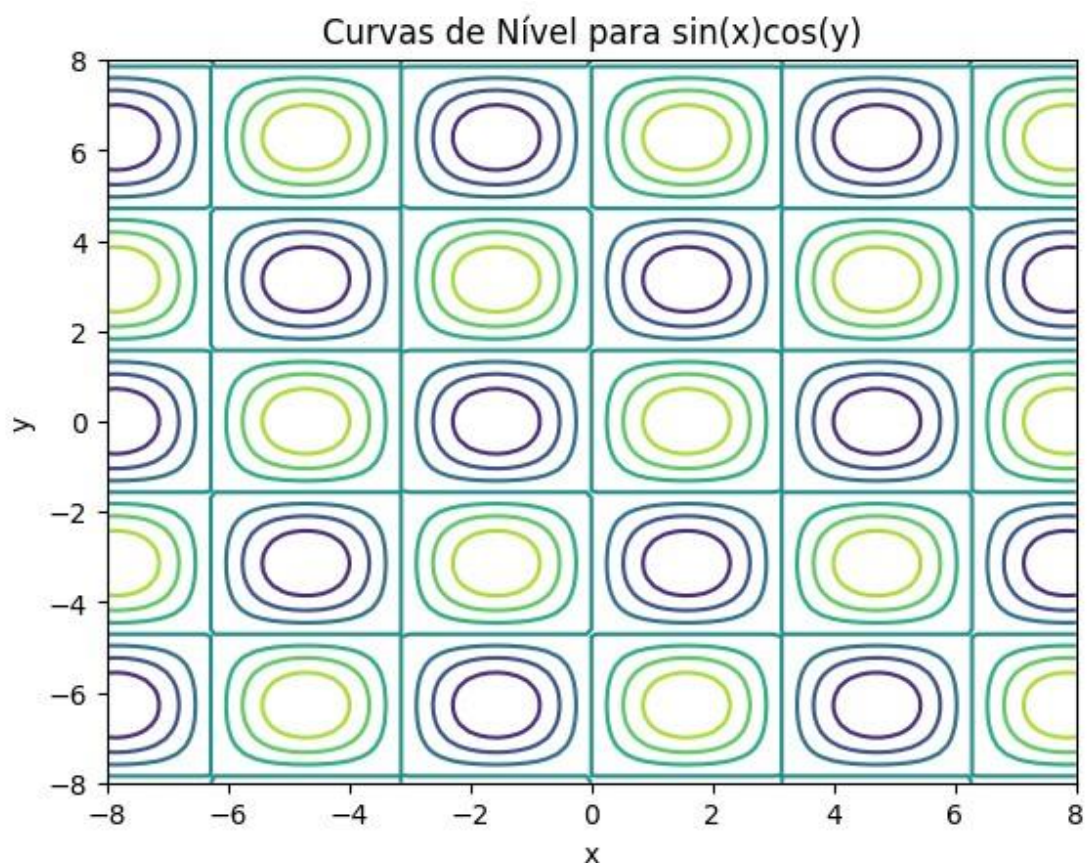
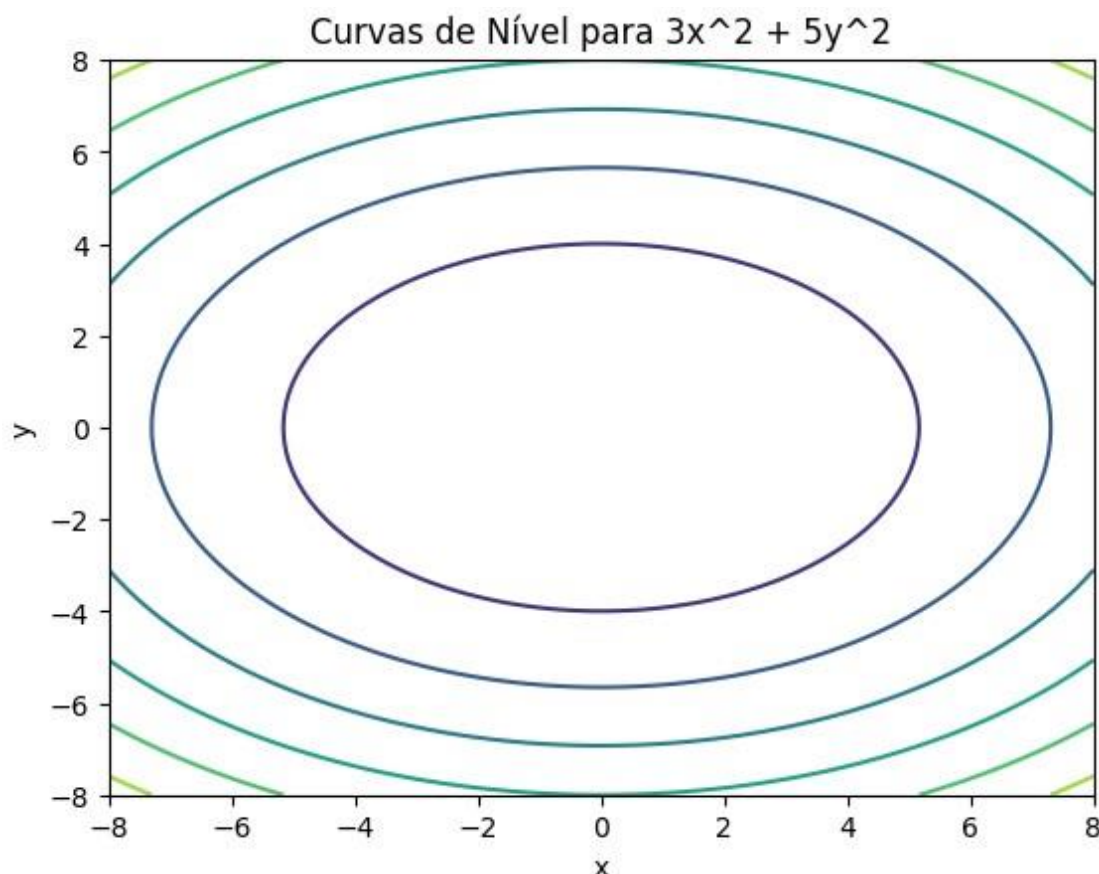


Gráfico 4:



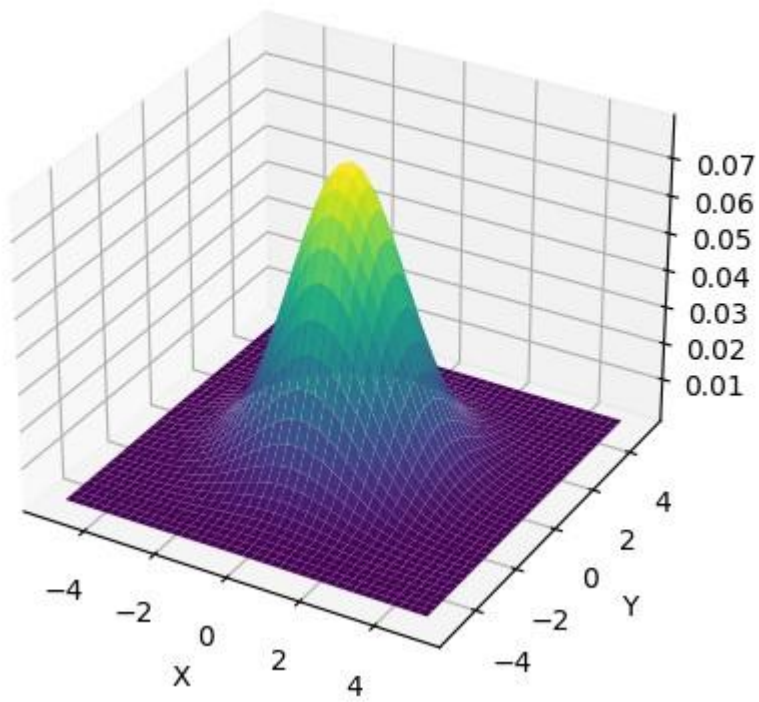
É possível notar nas primeiras curvas de nível os círculos diminuindo nos picos (máximos e mínimos) da onda formada pela função. Já na segunda vemos que as curvas de nível são elipses centradas na origem.

3 - b) Nesse caso foram elaborados 6 gráficos para instantes de tempo distintos $t=1,2,3,4,5$ e $t=10$. Para melhorar o entendimento desse fenômeno de espalhamento, esses gráficos foram elaborados no espaço cartesiano. O código criado e usando $t=1$ é mostrado a seguir:

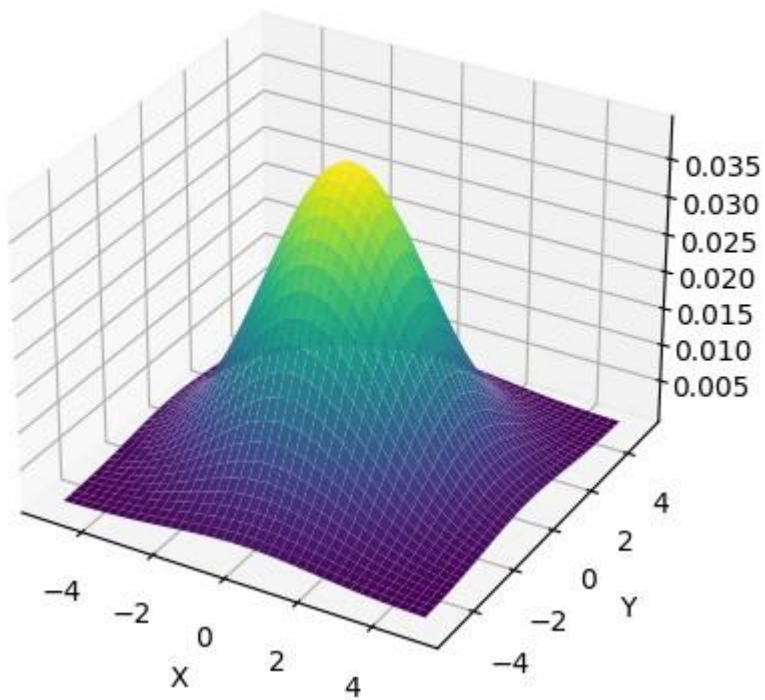
```
X, Y = np.meshgrid(np.arange(-5, 5.25, 0.25), np.arange(-5, 5.25, 0.25))
t = 1
z = (1/(4*np.pi*t)) * (np.exp((-X**2 - Y**2)/(4*t)))
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
surf = ax.plot_surface(X, Y, z, cmap='viridis')
ax.set_title("Espalhamento para t=1")
ax.set_xlabel("X")
ax.set_ylabel("Y")
ax.set_zlabel("Z")
plt.show()
```

Os resultados são mostrados nas figuras a seguir:

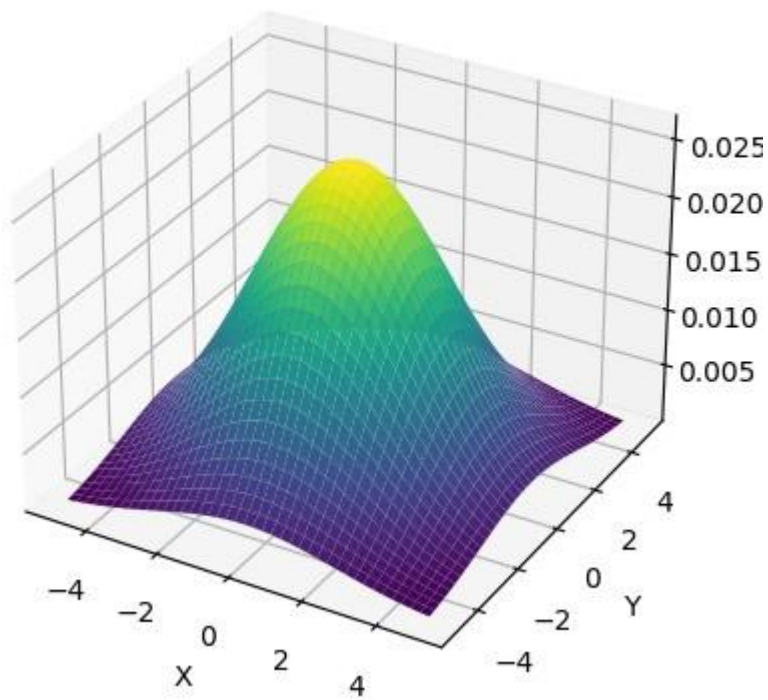
Espalhamento para $t=1$



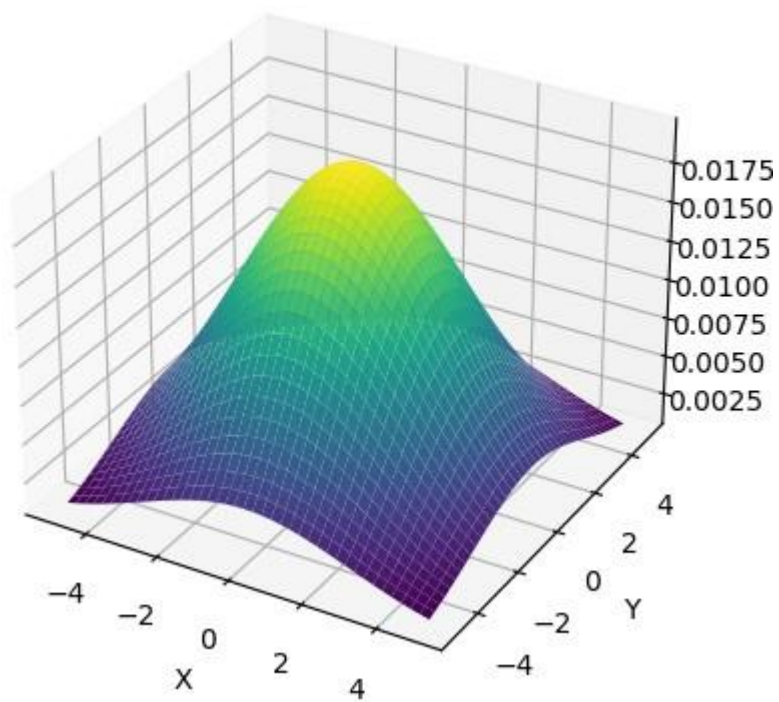
Espalhamento para $t=2$



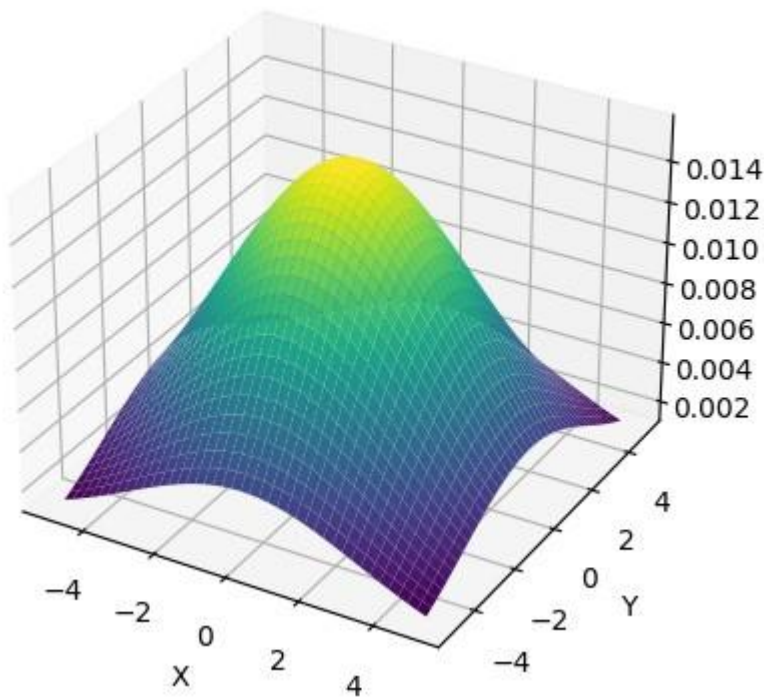
Espalhamento para $t=3$



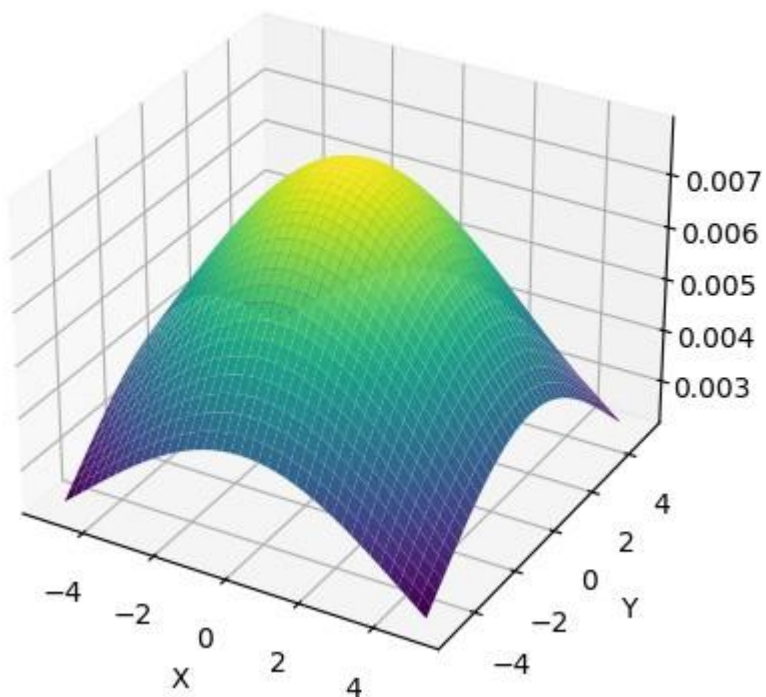
Espalhamento para $t=4$



Espalhamento para $t=5$



Espalhamento para $t=10$



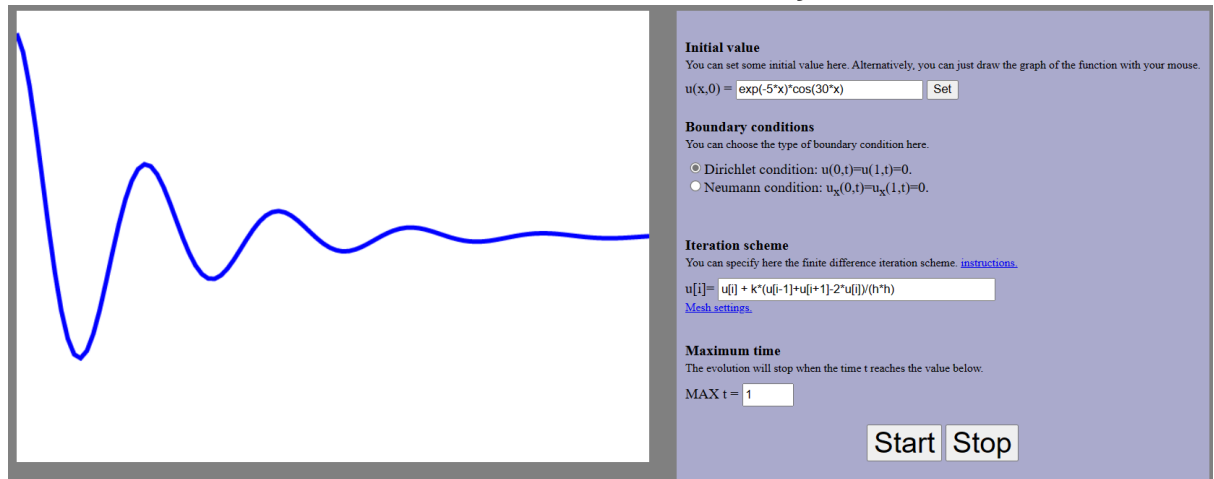
É fácil verificar a característica de fonte da distribuição, devido ao termo exponencial cujo argumento é $2t$, vê-se que quando o tempo cresce o espalhamento aumenta de maneira muito rápida.

Parte 2 - Diferenças Finitas e Simulações

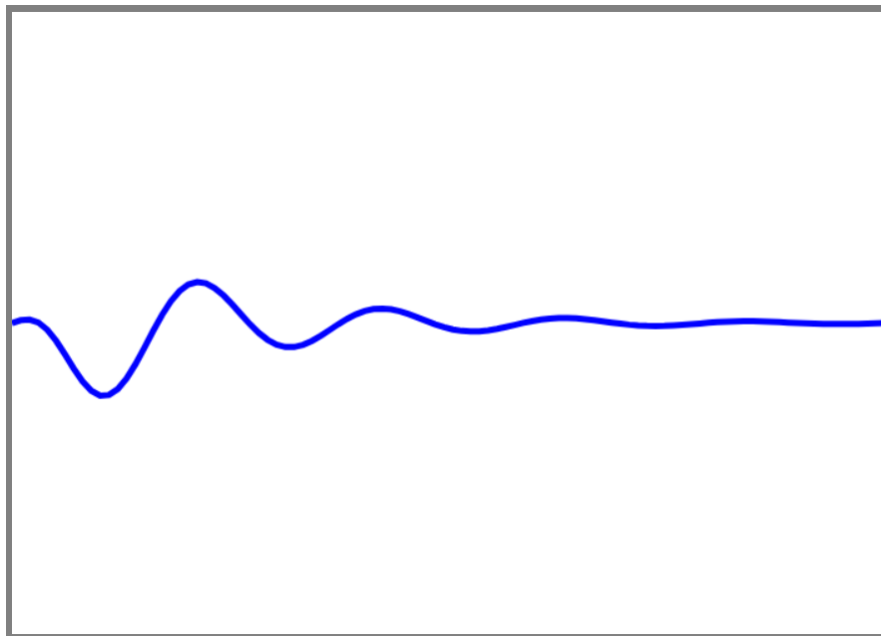
Inicialmente foram deduzidas todas as equações de diferenças finitas para cada modelo. As imagens obtidas em cada uma das simulações são mostradas a seguir (foram usadas apenas condições de Dirichlet):

1 - Difusão.

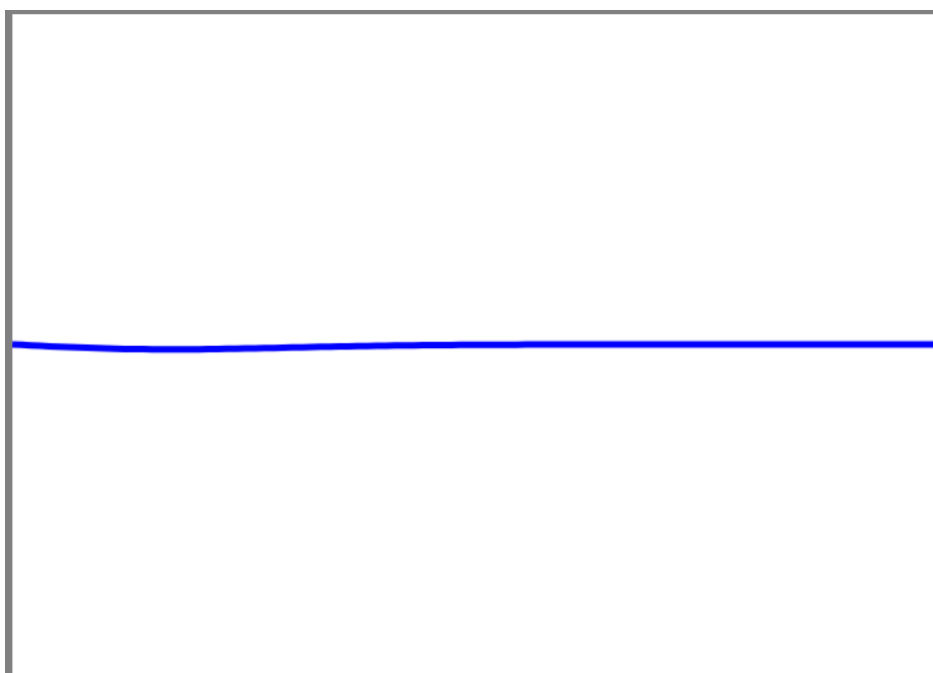
Perfil inicial usado em todas as simulações.



Meio da simulação.

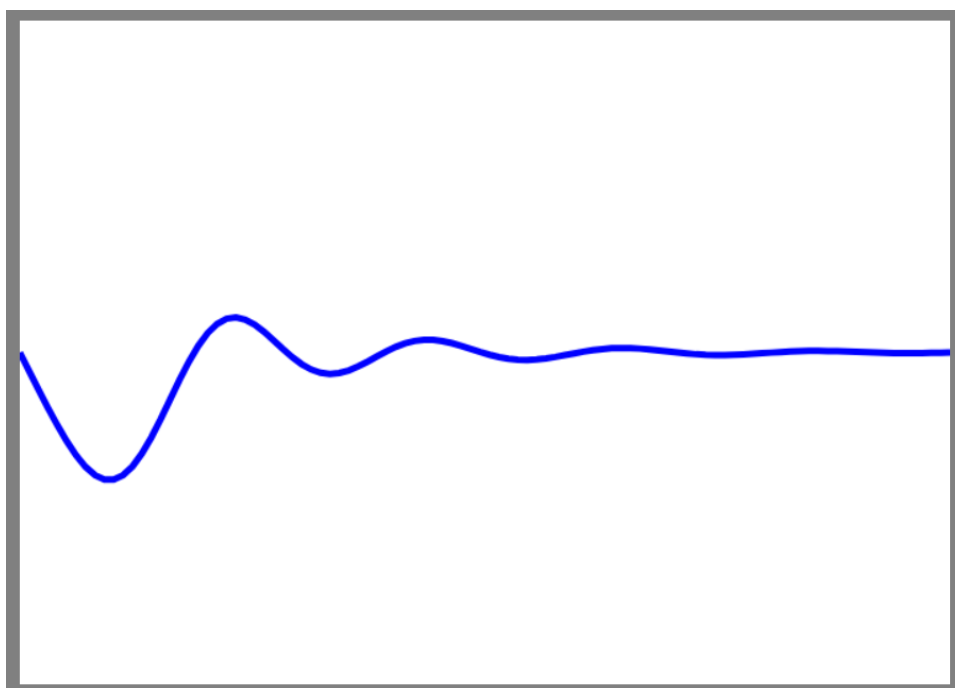


Final da Simulação.



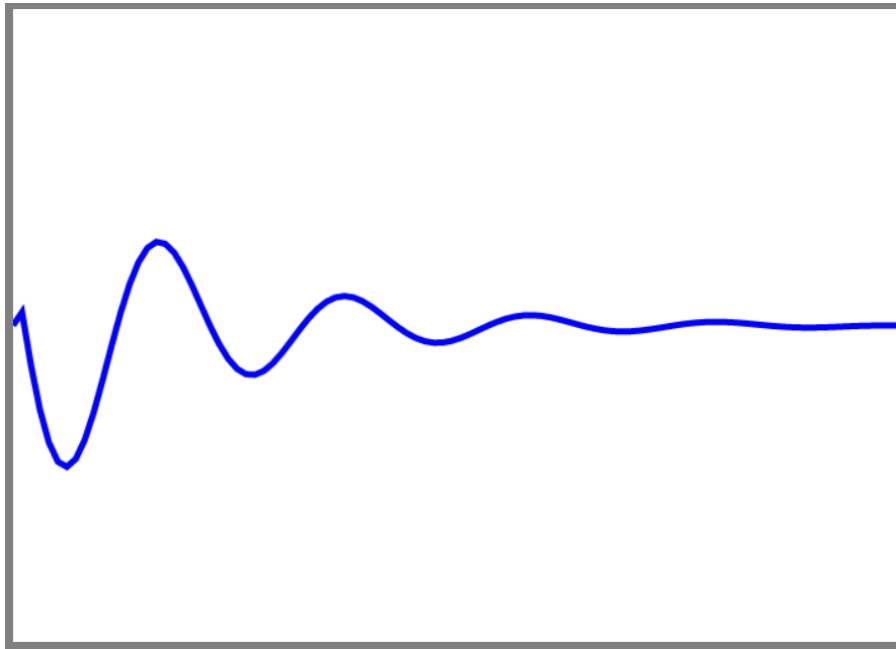
2 - Difusão - Reação.

Meio da simulação.



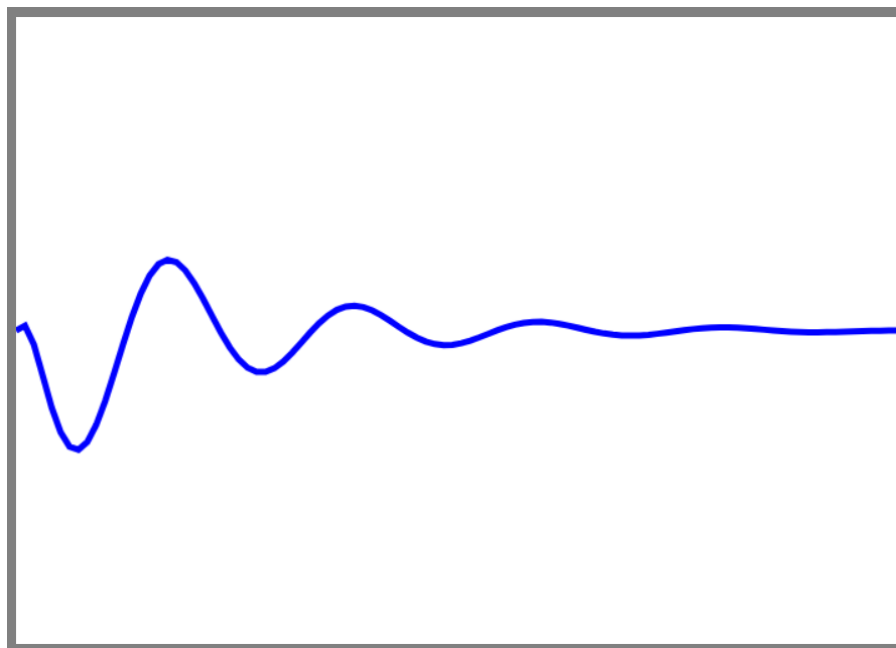
3 - Advecção.

Meio da simulação.



4 - Advecção - Difusão.

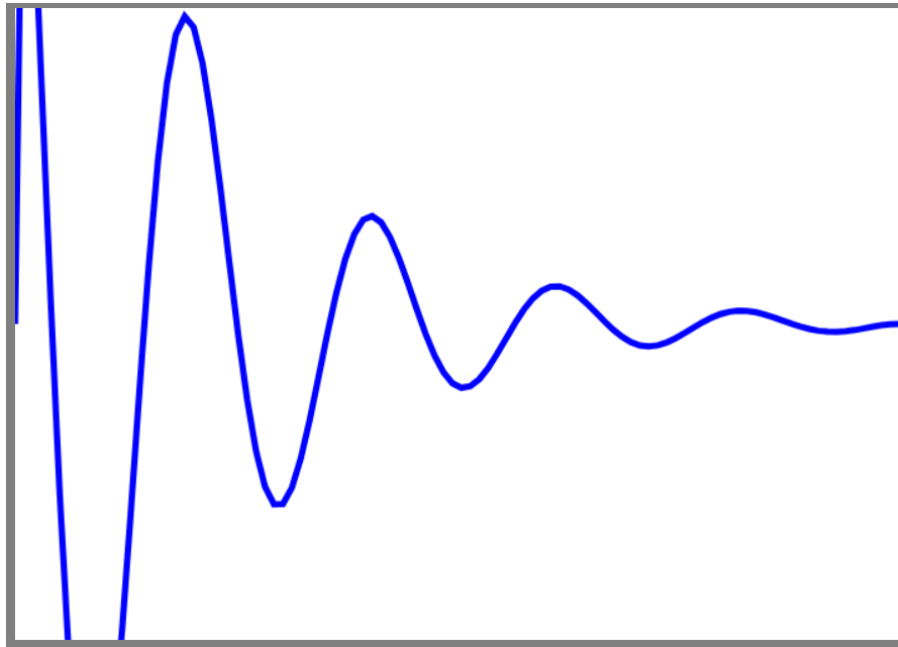
Meio da simulação.



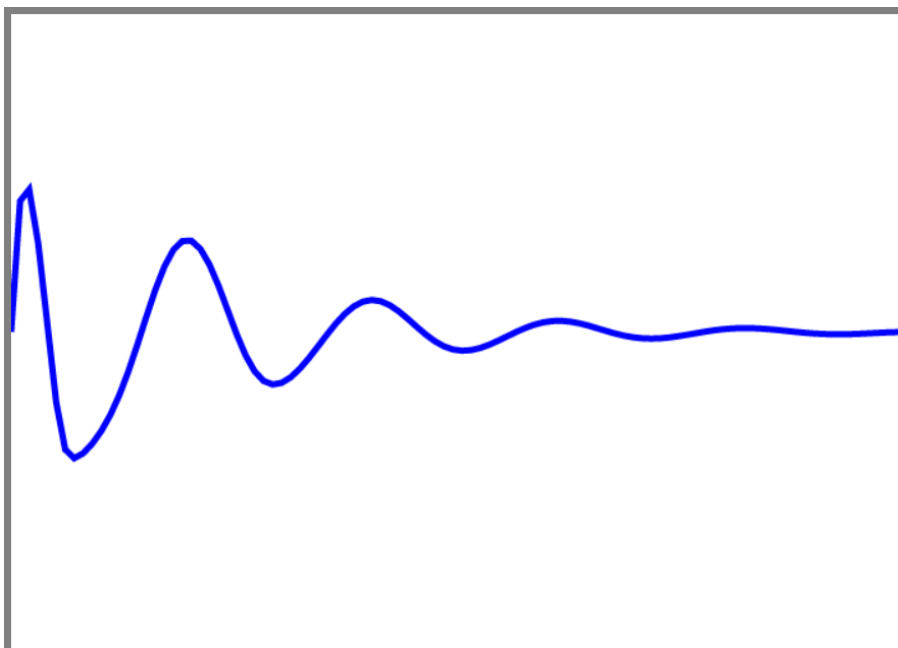
5 - Advecção - Reação.

Meio da simulação.

Como foi escolhido um termo de adição de substâncias, a solução explode quando o tempo tende ao infinito.



6 - Advecção - Reação - Difusão.



[Link dos códigos python com gráficos](#)