Approach 1: Diffusion Equation w Neumann B.C.

Governing Equation $\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2}, x \in (-\infty, +\infty)$

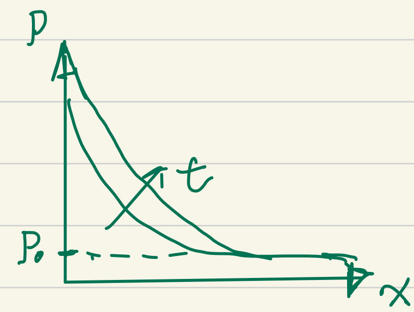
Darcy's Law
$Q = -\frac{k}{\mu}\frac{\partial P}{\partial x}$

Neumann B.C. $\frac{\partial P}{\partial x} = -\frac{\mu}{k}Q \quad x = 0^-$

$\frac{\partial P}{\partial x} = -\frac{\mu}{k}Q \quad x = 0^+$

Initial B.C. $P(x, 0) = P_0$

Simplify the problem by considering semi-infinite plane wall $x \in (0, +\infty)$



$$\begin{cases} \frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2} \\ \frac{\partial P}{\partial x} = -\frac{\mu}{k}Q \quad x = 0 \\ P(x, 0) = P_0 \\ P(\infty, t) = P_0 \end{cases}$$

Let $\theta = P - P_0$, then

$\theta(x, 0) = 0$

$\theta(\infty, t) = 0$

$\frac{\partial \theta}{\partial x} = -\frac{\mu}{k}Q$

Define Laplace transformation of a given pressure.

$$\mathcal{L}(P) = \int_0^\infty P\, e^{-st}\, dt$$

$$\mathcal{L}(P_0) = P_0 \int_0^\infty e^{-st}\, dt$$

$$= P_0 \left(-\frac{1}{s} e^{-st}\Big|_0^\infty\right)$$

$$= P_0 \left(-\frac{1}{s} \cdot -1\right) = \frac{P_0}{s}$$

$$\mathcal{L}\left(\frac{\partial P}{\partial t}\right) = \int_0^\infty \frac{\partial P}{\partial t}\, e^{-st}\, dt$$

$$\int_a^b u\, dV = u \cdot V\Big|_a^b - \int_a^b V\, du$$

$$u = e^{-st} \quad du = -se^{-st}$$

$$v = P \quad dv = \frac{dP}{dt} dt$$

$$= \int_0^\infty e^{-st}\, dP$$

$$= \left[e^{-st} P\right]_0^\infty - \int_0^\infty P(-s)\, e^{-st}\, dt$$

$$= \left[\cancel{e^{-st}} P\right]_{t=\infty} - \left[\overset{=1}{e^{-st}} P\right]_{t=0} + s\int_0^\infty P e^{-st} dt$$

$$= s\mathcal{L}(P) - P(x, 0)$$

$$= s\mathcal{L}(P) - P_0$$

$$\mathcal{L}\left(\frac{\partial P}{\partial x}\right) = \int_0^\infty \frac{\partial P}{\partial x}\, e^{-st} dt = \frac{\partial}{\partial x}\int_0^\infty P e^{-st} dt$$

$$= \frac{\partial \mathcal{L}(P)}{\partial x}$$

Similarly, we have Laplace transform relation for θ:

$$\mathcal{L}\left(\frac{\partial \theta}{\partial t}\right) = s\,\mathcal{L}(\theta) - \theta_0$$

$$\mathcal{L}\left(\frac{\partial^2 \theta}{\partial x^2}\right) = \frac{\partial^2 \mathcal{L}(\theta)}{\partial x^2}$$

Assume $\mathcal{L}(\theta) = \bar{\theta}$

Apply Laplace transform to diffusion equation

$$\mathcal{L}\left(\frac{\partial T}{\partial t}\right) = \mathcal{L}\left(D\frac{\partial^2 T}{\partial x^2}\right)$$

$$s\bar{\theta} - \theta_0 = D\frac{\partial^2 \bar{\theta}}{\partial x^2} \qquad (\theta_0 = 0)$$

$$\Rightarrow \frac{\partial^2 \bar{\theta}}{\partial x^2} - \frac{s}{D}\bar{\theta} = 0$$

Let $\bar{\theta} = e^{\lambda x}$

$$\left(\lambda^2 - \frac{s}{D}\right) e^{\lambda x} = 0$$

$$\lambda = \pm\sqrt{\frac{s}{D}}$$

$$\boxed{\bar{\theta} = A\,e^{\sqrt{s/D}\,x} + B\,e^{-\sqrt{s/D}\,x}}$$

Apply B.C. Laplace transform:

$$\bar{\theta}(\infty, s) = \mathcal{L}(\theta(\infty, t)) = 0 \qquad (1)$$

$$\frac{\partial \bar{\theta}(0,s)}{\partial x} = -\frac{\mu Q}{K s} \qquad (2)$$

Similar as $\mathcal{L}(P_0) = \frac{P_0}{s}$

From (1) $A = 0$

From (2)

$$\frac{\partial\bar{\theta}}{\partial x} = -\sqrt{s/D}\,B\,e^{-\sqrt{s/D}\cdot 0} = -\frac{\mu}{k}\frac{Q}{s}$$

$$B = \frac{\mu}{k}\frac{Q}{s\sqrt{s/D}}$$

$$\bar{\theta} = \frac{\mu Q}{k s\sqrt{s/D}}\, e^{-\sqrt{s/D}\,x}$$

Rearranging:

$$\boxed{\bar{\theta} = \frac{\mu Q\sqrt{D}/k}{s^{3/2}}\, e^{-(x/\sqrt{D})\sqrt{s}}}$$

Inverse Laplace Transform (Mathematica)

$$\theta = \frac{Q\mu}{k}\sqrt{D}\left[2\sqrt{\frac{t}{\pi}}\,e^{-\frac{x^2}{4Dt}} - \frac{x}{\sqrt{D}}\,\mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)\right]$$

$$\boxed{P = \frac{Q\mu}{k}\left[\sqrt{\frac{4Dt}{\pi}}\,e^{-\frac{x^2}{4Dt}} - x\,\mathrm{erfc}\left(\frac{x}{\sqrt{4Dt}}\right)\right]}$$

(assume $P_0 = 0$)

```
In[1]:= eqn = Exp[-(x / Sqrt[D]) * Sqrt[s]] * (mu * Q * Sqrt[D] / k) * s ^ (-3 / 2);
        InverseLaplaceTransform[eqn, s, t]
```

Out[2]=

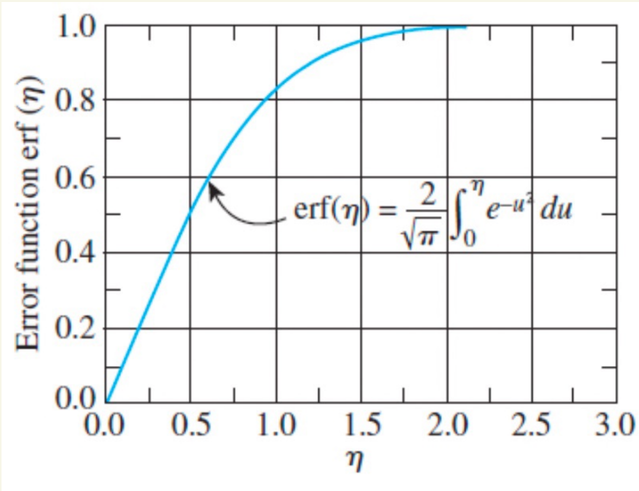
$$\frac{\sqrt{D}\ \mathrm{mu}\ Q\left(\frac{2 e^{-\frac{x^2}{4 D t}}\sqrt{t}}{\sqrt{\pi}} - \frac{x}{\sqrt{D}} + \frac{x\,\mathrm{Erf}\left[\frac{x}{2\sqrt{D t}}\right]}{\sqrt{D}}\right)}{k} \quad \text{if} \quad \frac{x}{\sqrt{D}} > 0$$

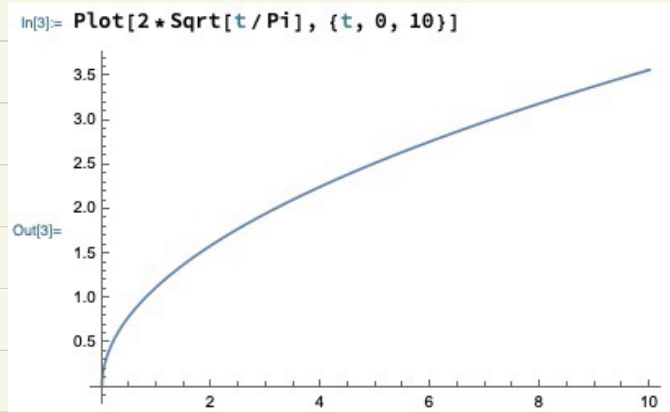
Notice: $1 - \mathrm{erf}(\eta) = \mathrm{erfc}(\eta)$

$\mathrm{erf}(\eta) = \frac{2}{\sqrt{\pi}}\int_0^{\eta} e^{-u^2}\,du$ Error Function

$\mathrm{erfc}(\eta) = 1 - \mathrm{erf}(\eta)$ Complementary Error Function

At injection point, $x = 0$
pressure scales like $p \propto 2\sqrt{\frac{t}{\pi}}$





Reference: Analytical Heat Transfer / Je-Chin Han
Example 4.3

Approach 2: Diffusion equation w source term.

Governing Equation: $\frac{\partial P}{\partial t} = D\frac{\partial^2 P}{\partial x^2} + S\,\delta(x)$ $\quad x \geq 0$

Boundary Condition: $P(\infty, t) = P_0$

Initial Condition: $P(x, 0) = P_0$

Apply Fourier Transform to the governing equation

$$\mathcal{F}\left[\frac{\partial P}{\partial t}\right] = \frac{\partial}{\partial t}\hat{P}$$

$$\mathcal{F}\left[\frac{\partial^2 P}{\partial x^2}\right] = (ik)^2\hat{P} = -k^2\hat{P}$$

$$\mathcal{F}[\delta(x)] = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\delta(x)\,e^{-ikx}\,dx$$

$$= \frac{1}{\sqrt{2\pi}}e^{-ik0} = \frac{1}{\sqrt{2\pi}}$$

Fourier Transform

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)\,e^{-ikx}\,dx$$

Inverse Fourier Transform

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\hat{f}(k)\,e^{ikx}\,dx$$

$$\frac{\partial\hat{P}}{\partial t} + \underbrace{Dk^2}_{C_1}\hat{P} = \underbrace{\frac{S}{\sqrt{2\pi}}}_{C_2}$$

Solving this ode use integrating factor

$$IF = e^{\int Dk^2\,dt} = e^{Dk^2 t}$$

Multiply both sides by e^{Dk^2t}

$$e^{Dk^2t}\left(\frac{\partial \hat{p}}{\partial t} + Dk^2\hat{p}\right) = e^{Dk^2t}\frac{S}{\sqrt{2\pi}}$$

use product rule, this is just

$$\frac{d}{dt}\left(\hat{p}\, e^{Dk^2t}\right) = \frac{S}{\sqrt{2\pi}}e^{Dk^2t}$$

Integrate both sides from 0 to t

$$\frac{d}{dt}\left(\hat{p}\, e^{Dk^2t}\right) = \frac{S}{\sqrt{2\pi}}\int_0^t e^{Dk^2\tilde{t}}\, d\tilde{t}$$

$$\text{RHS}: \frac{S}{\sqrt{2\pi}}\frac{1}{Dk^2}\left[e^{Dk^2\tilde{t}}\right]_{\tilde{t}=0}^{\tilde{t}=t}$$

$$\hat{p} = \frac{S}{\sqrt{2\pi}}\frac{1}{Dk^2}\left[1 - e^{-Dk^2t}\right] + Ce^{-Dk^2t}$$

$$\hat{p}(x,0) = 0$$

$$C = 0$$

$$\hat{p} = \frac{S}{\sqrt{2\pi}}\frac{1}{Dk^2}\left[1 - e^{-Dk^2t}\right]$$

Inverse Fourier Transform.

$$\boxed{\hat{p} = \left[\sqrt{\frac{t}{D\pi}}\, e^{-\frac{x^2}{4Dt}} - \frac{1}{2D}x\, \mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)\right]S}$$

where: $D = \dfrac{k}{\mu\phi C_t}$

$S = \dfrac{\tilde{m}}{\rho\phi C_t}$

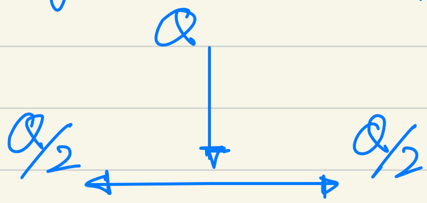
```
In[57]:= InverseFourierTransform[S / Sqrt[2 * Pi] * 1 / (D * k ^ 2) * (1 - Exp[-D * k ^ 2 * t]), k, x]
```

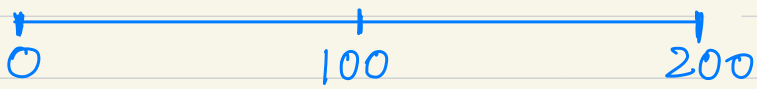
Out[57]= $$\frac{S\left(2e^{-\frac{x^2}{4Dt}}\sqrt{Dt} + \sqrt{\pi}\,\mathrm{Abs}[x]\,\mathrm{Erf}\left[\frac{\mathrm{Abs}[x]}{2\sqrt{Dt}}\right] - \sqrt{\pi}\,x\,\mathrm{Sign}[x]\right)}{2D\sqrt{\pi}}$$

Numerical Simulation of Diffusion equation w injection.

Approach 1: Neumann Boundary Condition.

only simulate half domain and use symmetry





$$\frac{Q}{2} = -\frac{k}{\mu}\frac{P_{n+1}-P_n}{\Delta x}$$

$$Q = \left(\frac{-2k}{\mu\Delta x}\right)P_{n+1} + \left(\frac{2k}{\mu\Delta x}\right)P_n$$

Applied at $x=0$ as boundary condition.

At the point of injection, introduce ghost node for central difference.

$$\frac{\partial P}{\partial x}(0,t) = \underbrace{-\frac{\mu}{k}\frac{Q}{2}}_{C}$$

$$\frac{P(0+\Delta x,t)-P(0-\Delta x,t)}{2\Delta x} = C$$

$$P(-\Delta x,t) = P(\Delta x,t) - 2\Delta x C \Rightarrow P_{-1} = P_1 - 2\Delta x C$$

use this relation to insert central difference for this node:

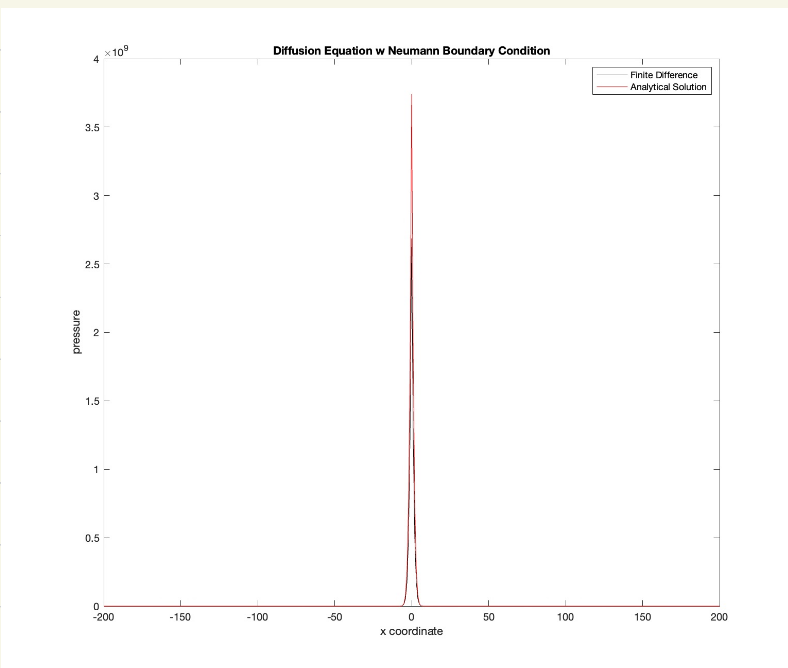
$$\frac{P_1 - 2P_0 + P_{-1}}{\Delta x^2} = \frac{2P_1 - 2P_0 - 2\Delta x C}{\Delta x^2}$$

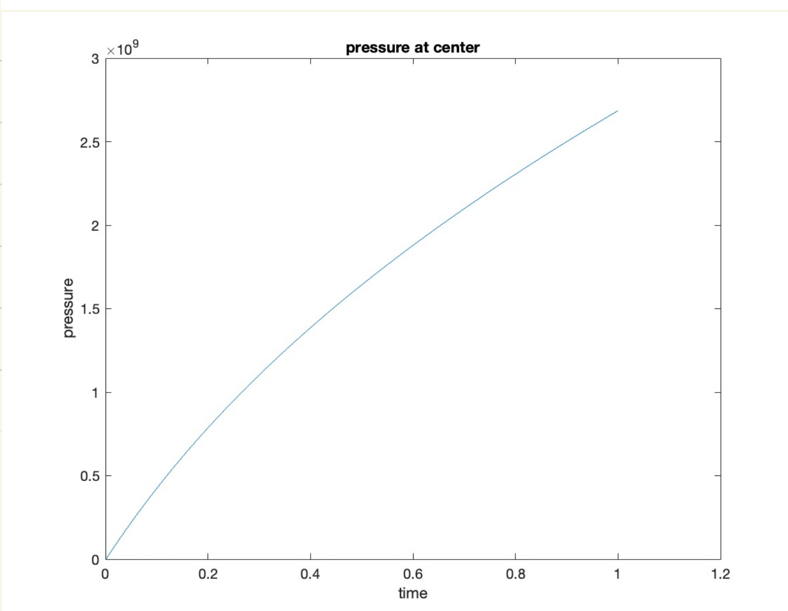
$$\boxed{= \left(\frac{2}{\Delta x^2}\right) P_1 - \left(\frac{2}{\Delta x^2}\right) P_0 \underbrace{- \frac{2C}{\Delta x}}_{+\frac{\cancel{2}}{\Delta x}\frac{\mu}{k}\frac{Q}{\cancel{2}}}}$$

use symmetry to obtain the spatial distribution of pressure profile.

- Previously, the one-sided discretization is only first-order accuracy.

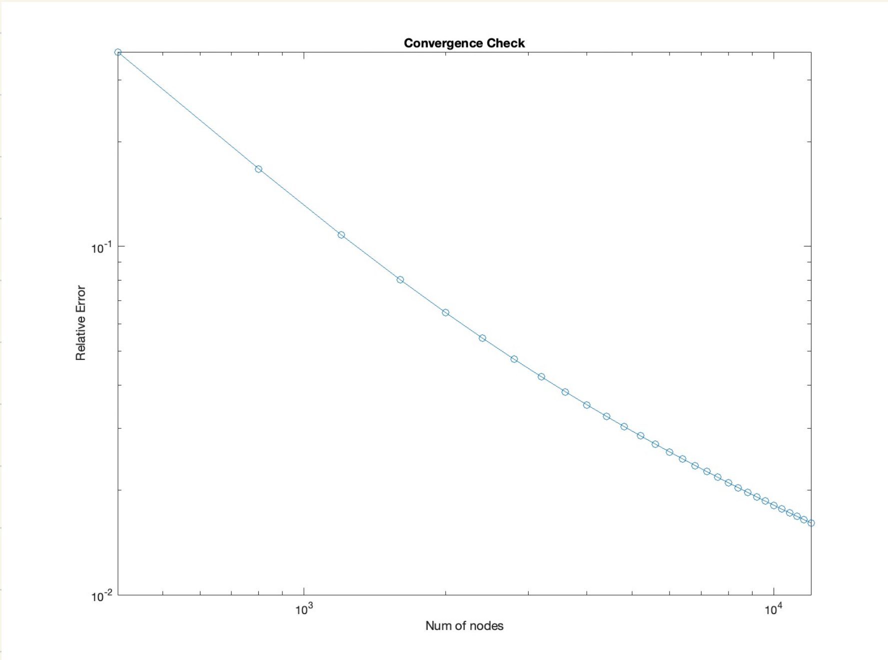
Simulate to $t = 1s$.





- key points:
(1) Simulate half of domain & impose symmetry
(2) Second-order finite difference w ghost nodes.

Convergence Check: log-log plot of relative error v.s. number of nodes. (at time $t=1s$)



The relative error is computed nodal-wise:

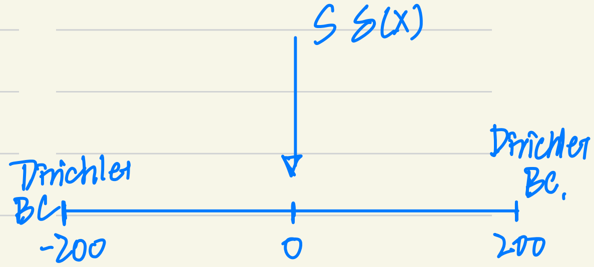
$$REr r = \sqrt{\sum_i (f_i - g_i)\,\Delta X}$$

f_i := numerical value at point i

g_i := analytical value at point i

ΔX := interval distance.

Approach 2: Point Source term



Consider whole simulation domain.

$$\underbrace{\frac{\partial P}{\partial t}}_{\substack{\text{RK4} \\ | \\ \text{(ode45)}}} = D\underbrace{\frac{\partial^2 P}{\partial x^2}}_{\substack{\text{central} \\ \text{difference}}} + S\,\delta(x)$$

key point: approximate $\delta(x)$ function w second-order difference

$$\tilde{\delta}_i = \tilde{\delta}_i^+ + \tilde{\delta}_i^-$$

and:

$$\tilde{\delta}_i^+ = \begin{cases} (x_{i+1}-\alpha)/h^2 & \text{if} \quad x_i \leqslant \alpha < x_{i+1}, \\ 0, & \text{otherwise,} \end{cases}$$

$$\tilde{\delta}_i^- = \begin{cases} (\alpha - x_{i-1})/h^2 & \text{if} \quad x_{i-1} < \alpha < x_i, \\ 0, & \text{otherwise.} \end{cases}$$

Reference:

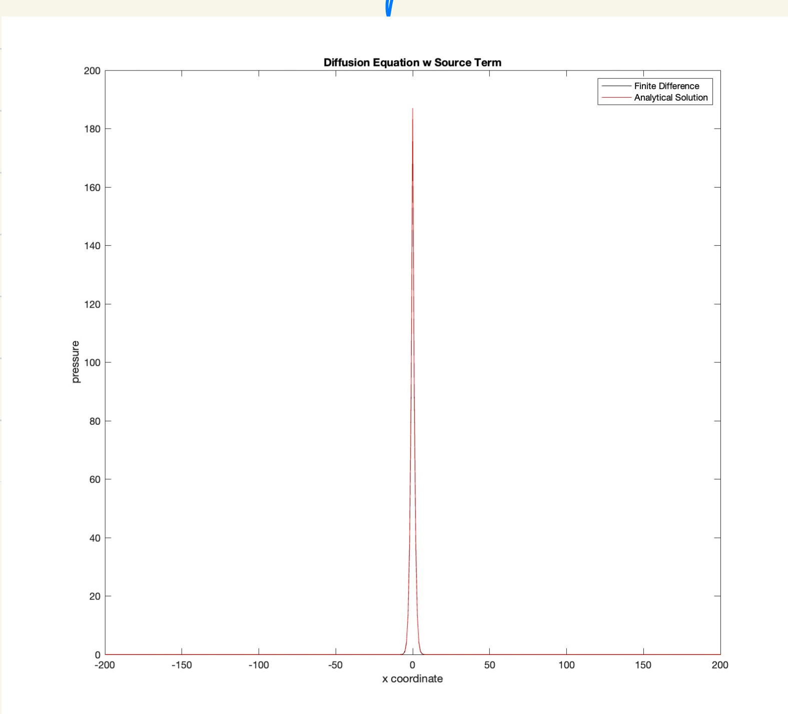
The numerical approximation of a delta function with application to level set methods

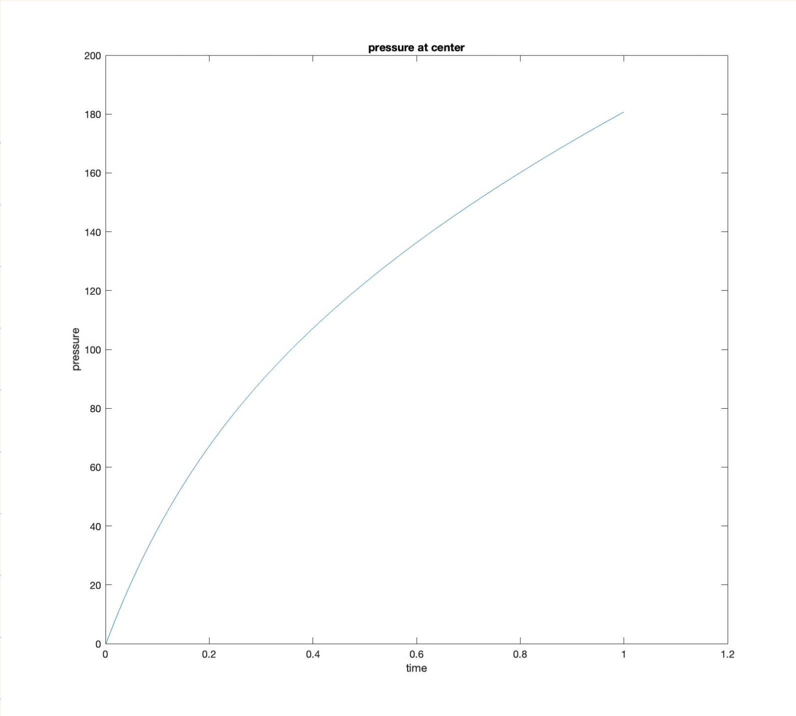
Peter Smereka *

In this case, the $\delta(x)$ approximation becomes $\frac{1}{dx}$ $(\alpha = x_i)$

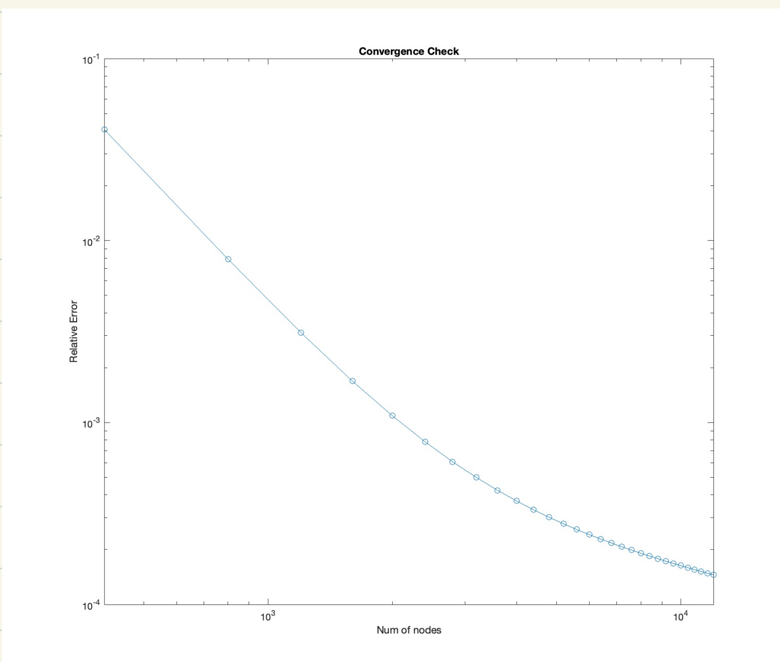
$$\left(\frac{\partial P}{\partial t}\right)_{RK4} = D\frac{P_{n+1} - 2P_n + P_{n-1}}{\Delta x^2} + \left(S\,\frac{1}{dx}\right)_{x=0}$$

Simulate the system to $t = 1s$





Convergence Analysis. similar to approach 1, we plot relative error v.s. number of nodes (at time t=1s)



The relative error is computed nodal-wise:

$$RErr = \sqrt{\sum_i (f_i - g_i)\Delta X}$$

f_i := numerical value at point i

g_i := analytical value at point i

ΔX := interval distance.