



A Hands-On Introduction to Computational Fluid Dynamics

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FLOW

SERC
Swedish e-Science Research Centre

Computational Fluid Dynamics

17th Century
France and England

PURE
EXPERIMENTS

Computational Fluid Dynamics

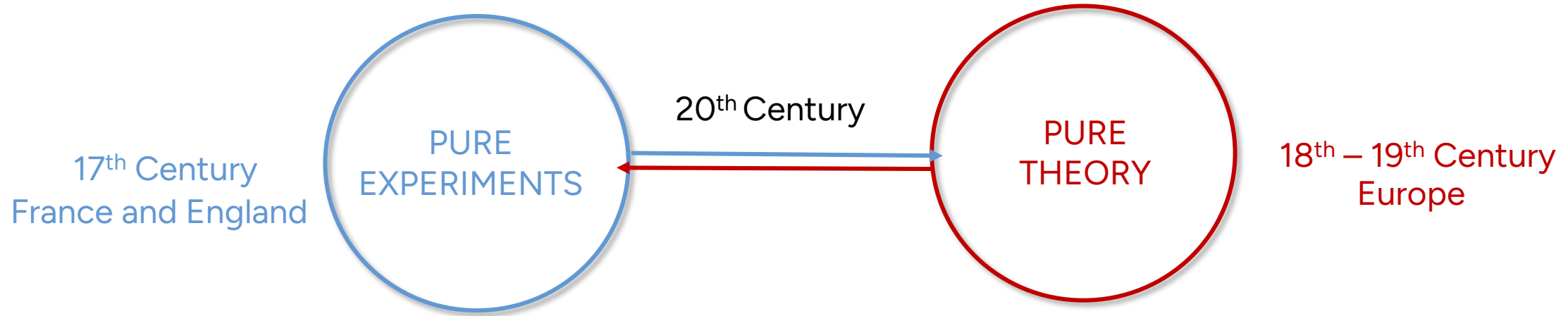
17th Century
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PURE
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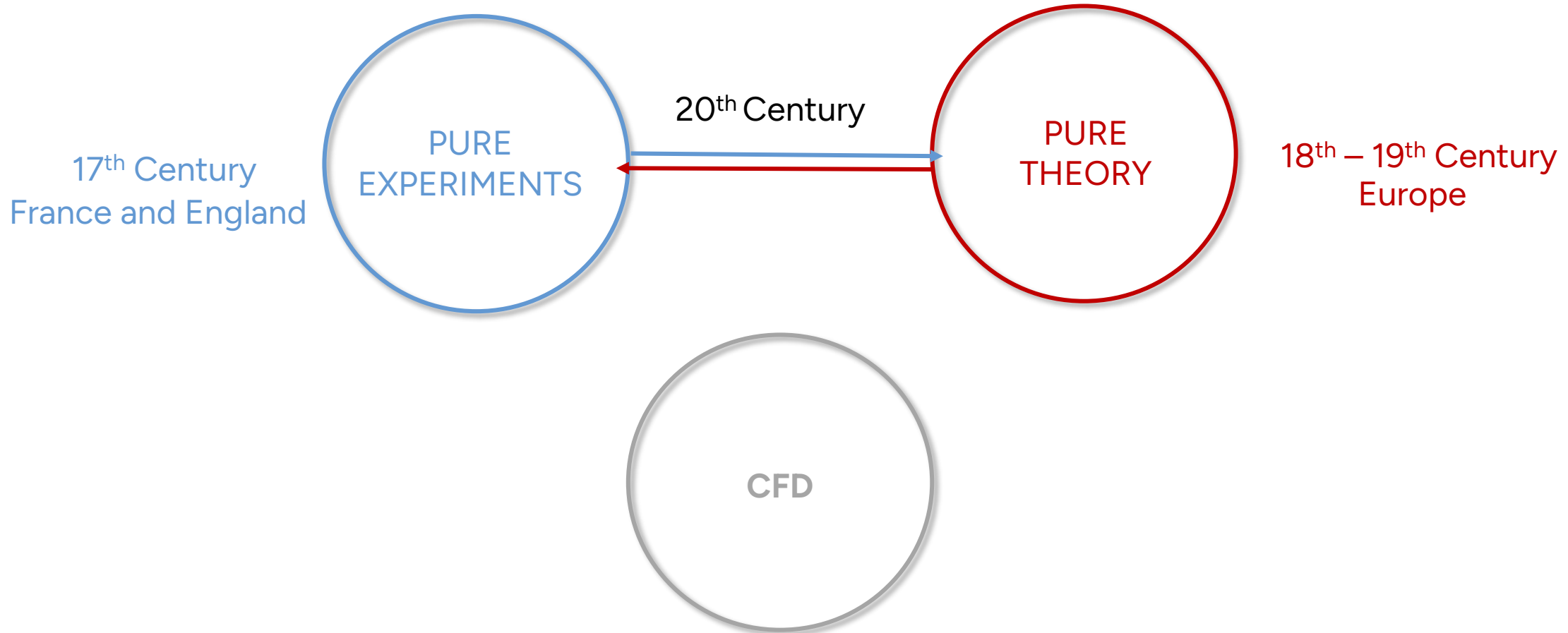
PURE
THEORY

18th – 19th Century
Europe

Computational Fluid Dynamics

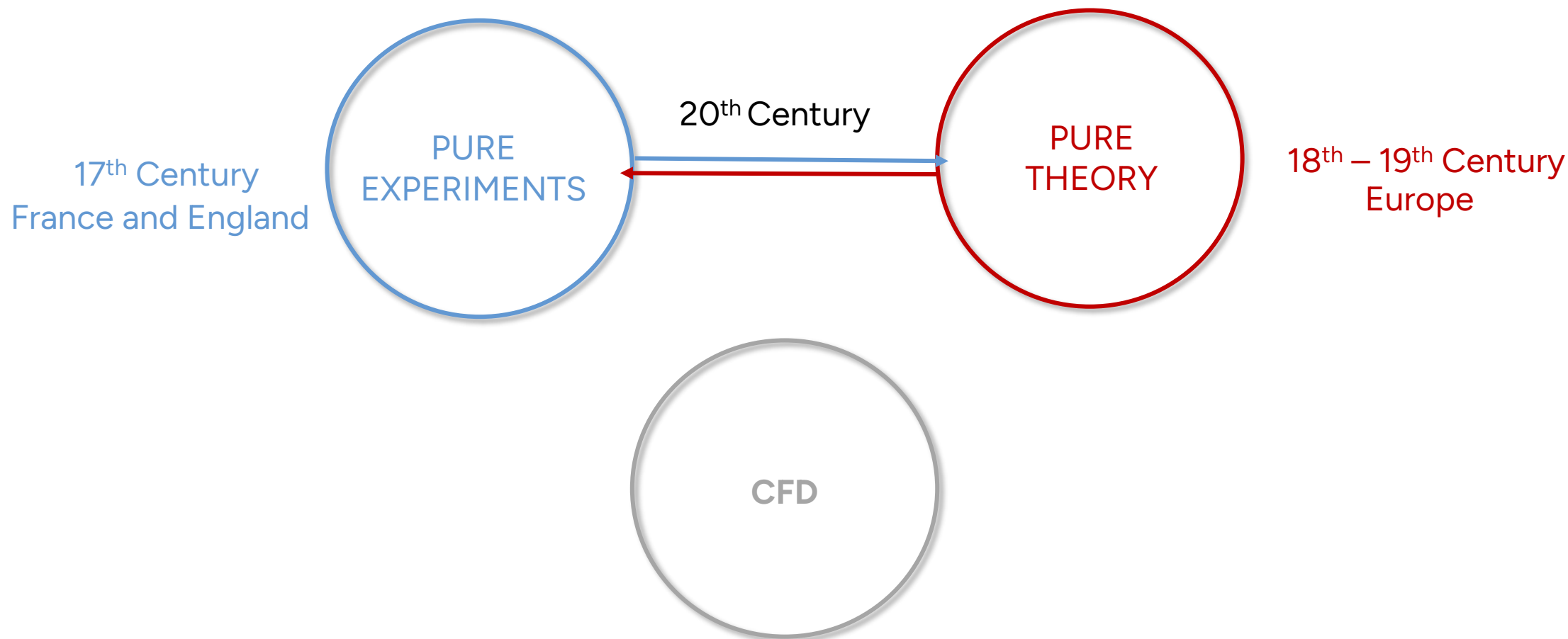


Computational Fluid Dynamics



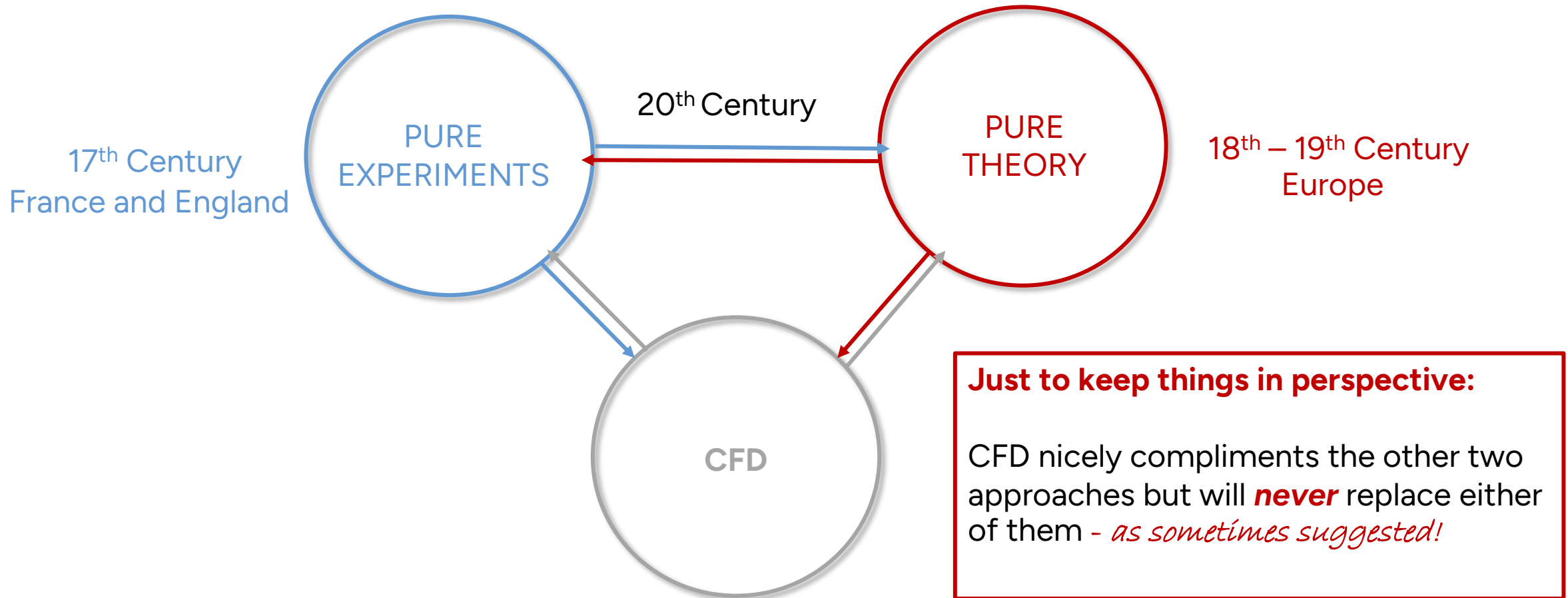
A new *“third approach”* in the philosophical study of fluid dynamics

Computational Fluid Dynamics



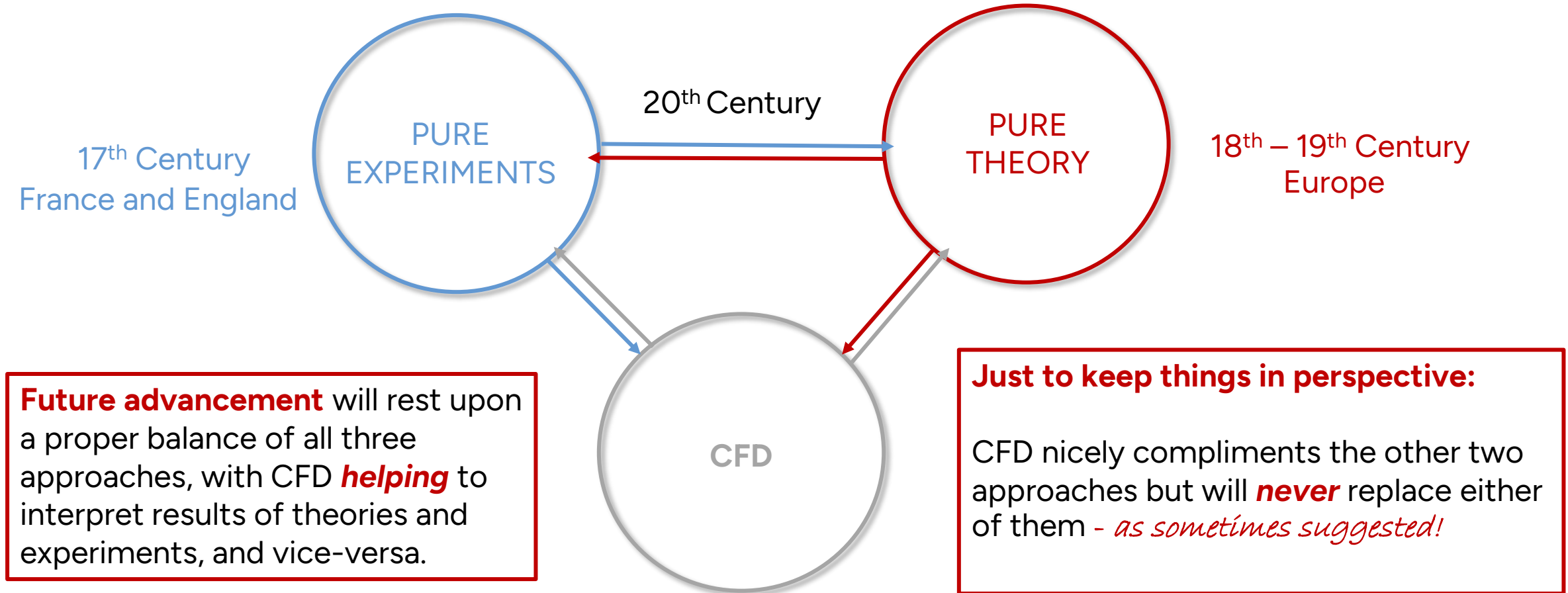
A new *“third approach”* in the philosophical study of fluid dynamics
(*Nothing more than that!*)

Computational Fluid Dynamics



A new “third approach” in the philosophical study of fluid dynamics
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Computational Fluid Dynamics



A new "third approach" in the philosophical study of fluid dynamics
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CFD as a research tool



CFD results are directly analogous to Wind Tunnel results.

However, unlike a wind tunnel a computer program can be carried everywhere or can be accessed sitting *1000 miles away!*

A CFD program is, therefore, a *"readily transportable wind tunnel"*, where you can carry out *"numerical experiments"*.

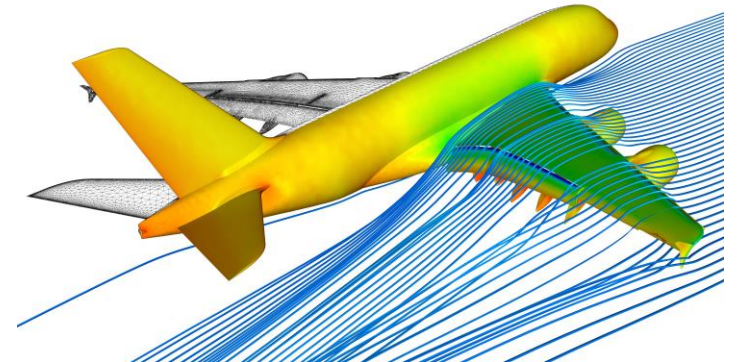


CFD as a research tool: Who cares?



CFD as a research tool: Who cares?

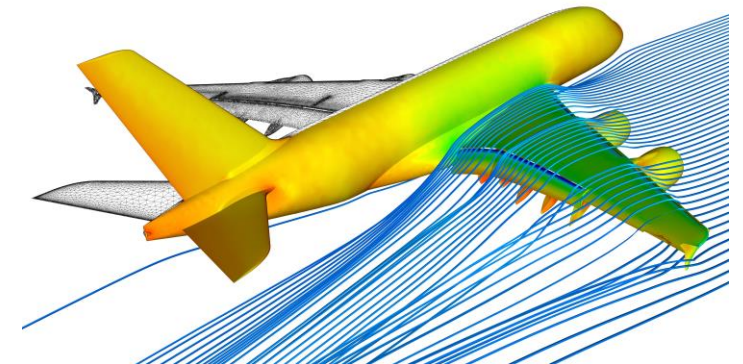
Aviation



CFD as a research tool: Who cares?



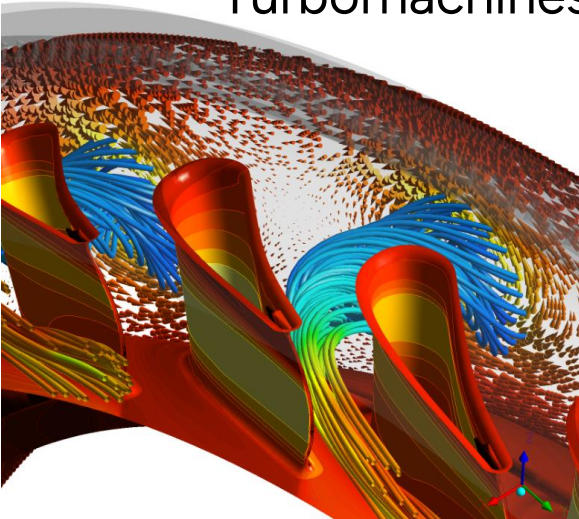
Automotive



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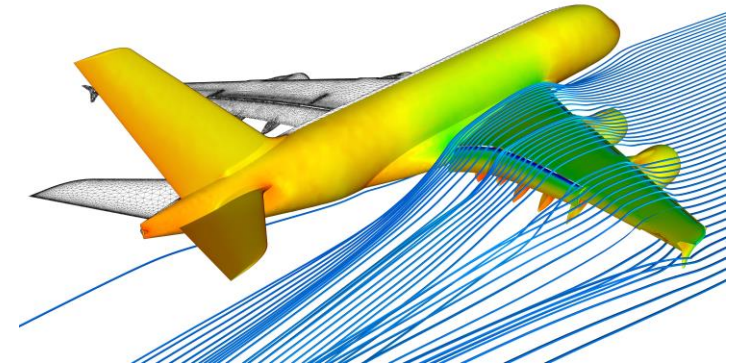
Turbomachines



Automotive

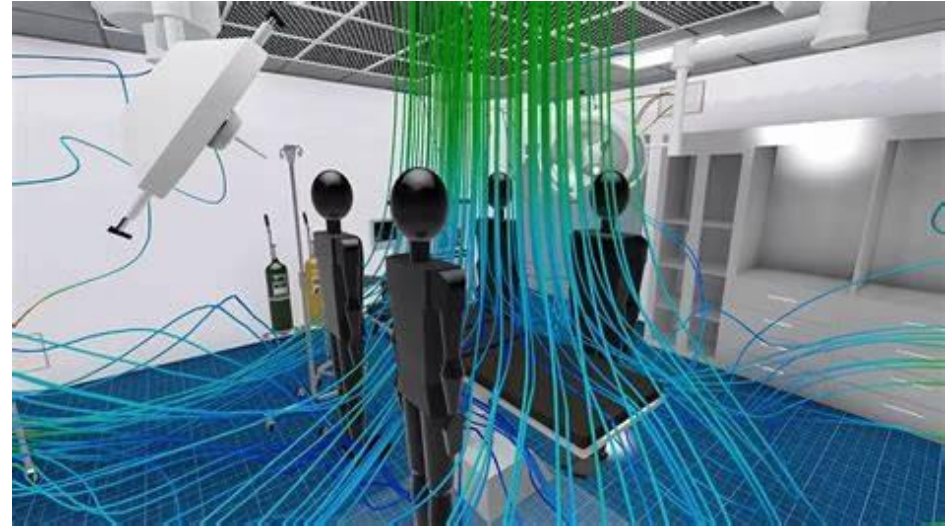


Aviation

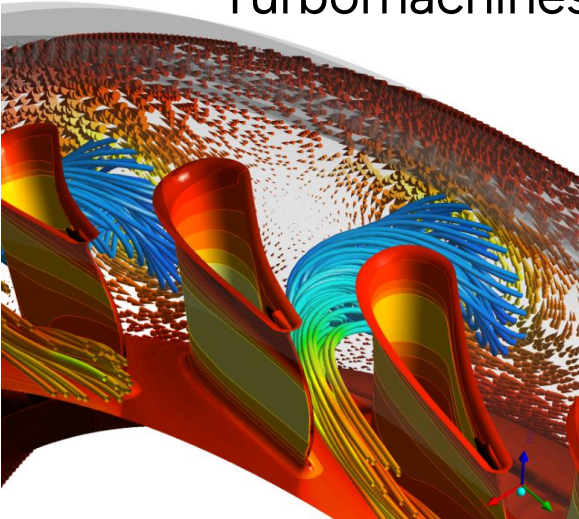


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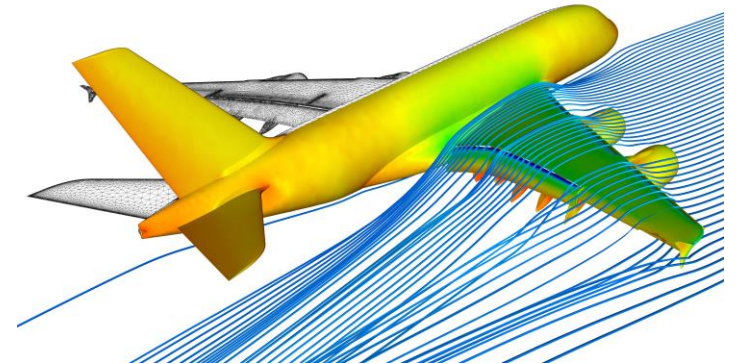
HVAC



Turbomachines



Aviation

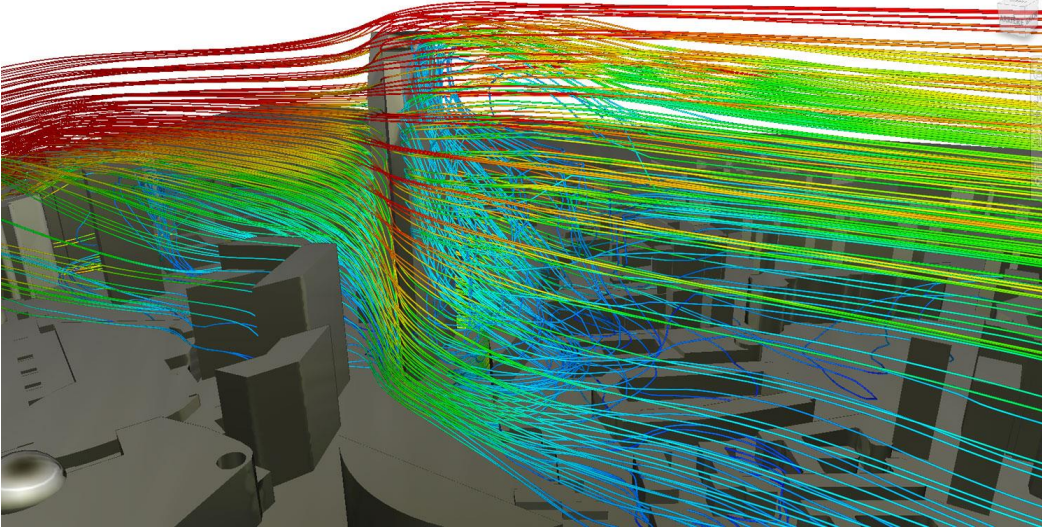


Automotive

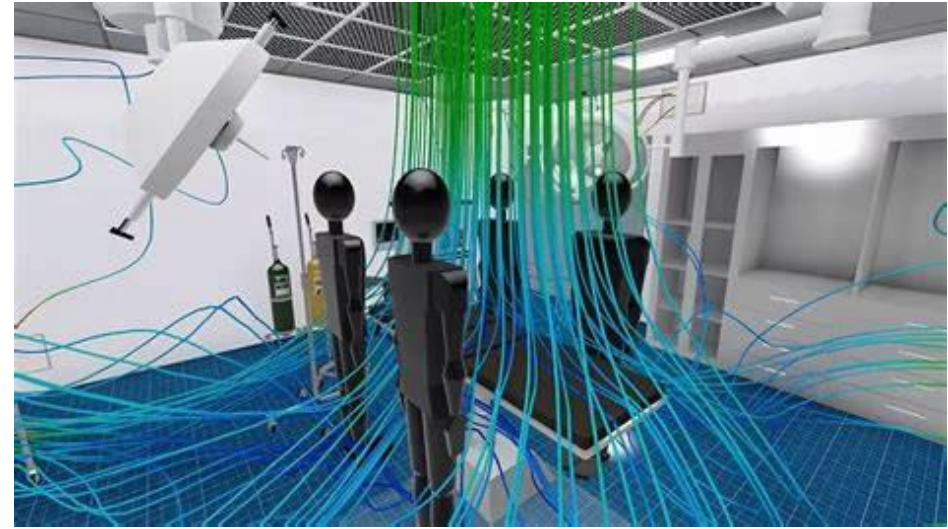


CFD as a research tool: Who cares?

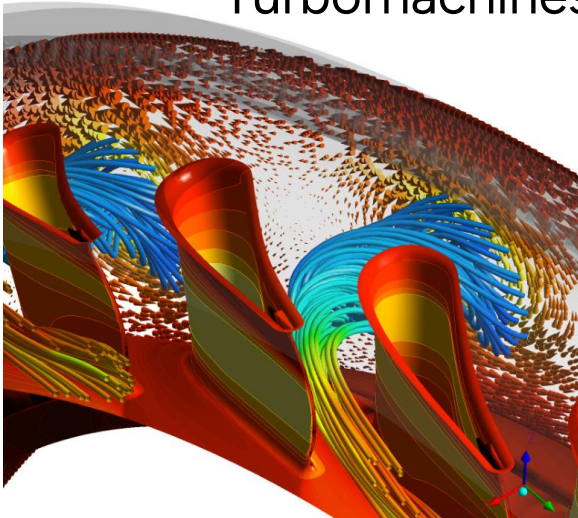
Cities



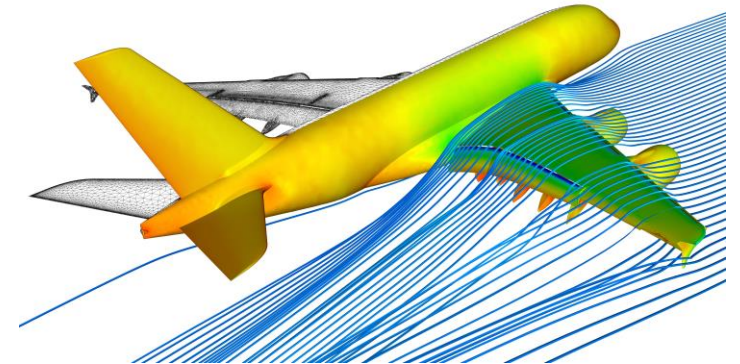
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Turbomachines



Aviation

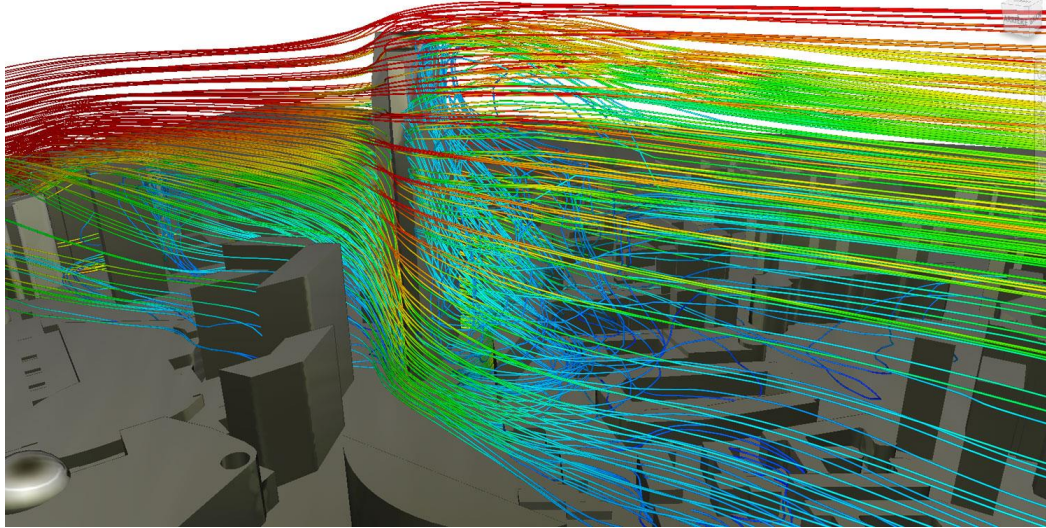


Automotive

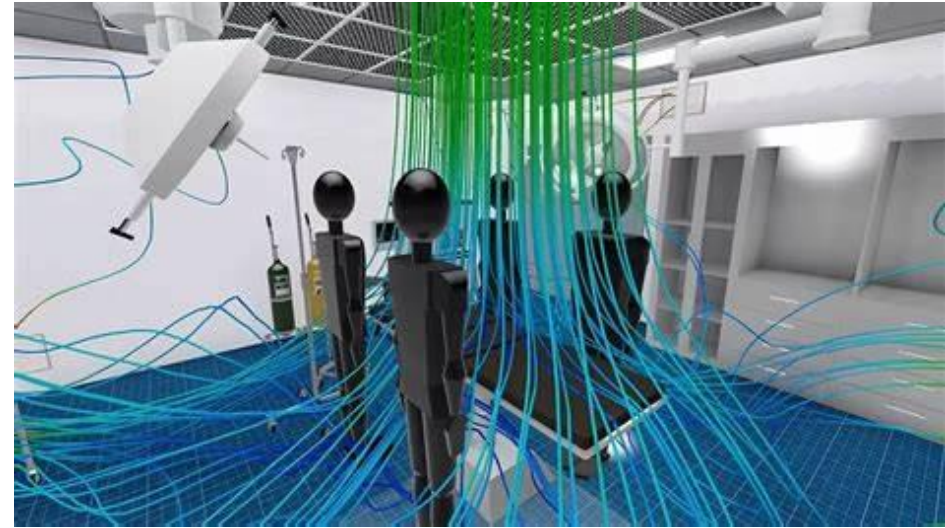


CFD as a research tool: Who cares?

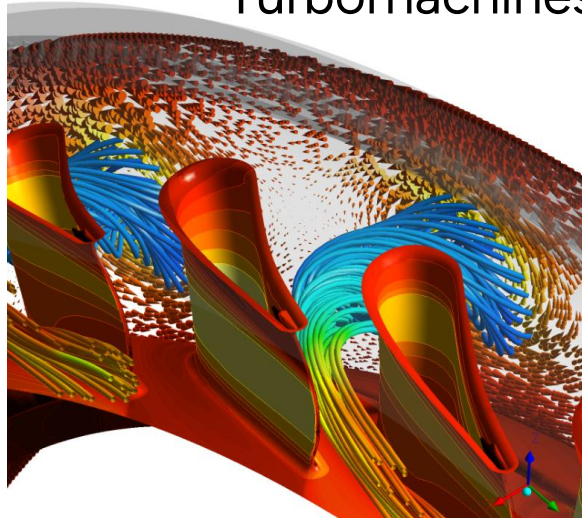
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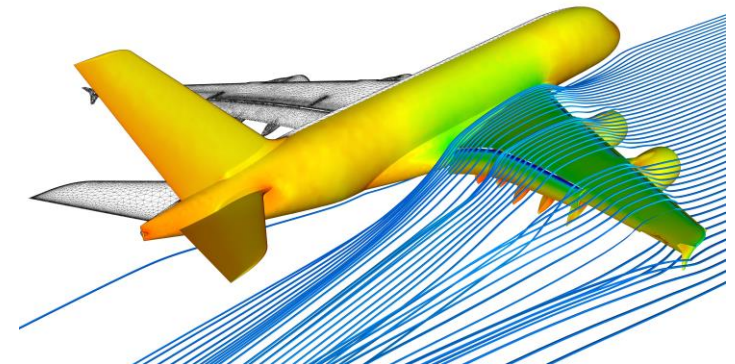
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Automotive



+ many more !

So How to CFD?

CFD involves:

- Identifying the physical phenomenon, that includes Governing equations, Initial & Boundary conditions.
- Breaking down the continuous problem to a discrete representation.
- Solving the discrete set of equations using adequate numerical methods.
- Post processing the results.

THE GRAND CHALLENGE EQUATIONS

$$\begin{aligned}
 & B_i A_i = E_i A_i + \rho_i \sum_j B_j A_j F_{ji} & \nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} & \vec{F} = m \vec{a} + \frac{dm}{dt} \vec{v} \\
 & dU = \left(\frac{\partial U}{\partial S} \right)_V dS + \left(\frac{\partial U}{\partial V} \right)_S dV & \nabla \cdot \vec{D} = \rho & Z = \sum_j g_j e^{-E_j/kT} \\
 & F_j = \sum_{k=0}^{N-1} f_k e^{2\pi i j k / N} & \nabla^2 u = \frac{\partial u}{\partial t} & \nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} + \vec{J} \\
 & & p_{n+1} = r p_n (1 - p_n) & \nabla \cdot \vec{B} = 0 & P(t) = \frac{\sum_i W_i B_i(t) P_i}{\sum_i W_i B_i(t)} \\
 & -\frac{\hbar^2}{8\pi^2 m} \nabla^2 \Psi(r, t) + V \Psi(r, t) = -\frac{\hbar}{2\pi i} \frac{\partial \Psi(r, t)}{\partial t} & & -\nabla^2 u + \lambda u = f \\
 & \frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = -\frac{1}{\rho} \nabla p + \gamma \nabla^2 \vec{u} + \frac{1}{\rho} \vec{F} & \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = f
 \end{aligned}$$

• NEWTON'S EQUATIONS • SCHROEDINGER EQUATION (TIME DEPENDENT) • NAVIER-STOKES EQUATION •
 • POISSON EQUATION • HEAT EQUATION • HELMHOLTZ EQUATION • DISCRETE FOURIER TRANSFORM •
 • MAXWELL'S EQUATIONS • PARTITION FUNCTION • POPULATION DYNAMICS •
 • COMBINED 1ST AND 2ND LAWS OF THERMODYNAMICS • RADIOSITY • RATIONAL B-SPLINE •

What are we solving?

Navier Stokes equations

Continuity equation: $\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$

Momentum equation: $\partial_t \rho \mathbf{u} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p - \nabla \cdot \boldsymbol{\tau} = \mathbf{f}$

Energy equation: $\partial_t E + \nabla \cdot [(E + p)\mathbf{u}] - \nabla \cdot (\boldsymbol{\tau} \mathbf{u}) - \nabla \cdot (\kappa \nabla T) = S$

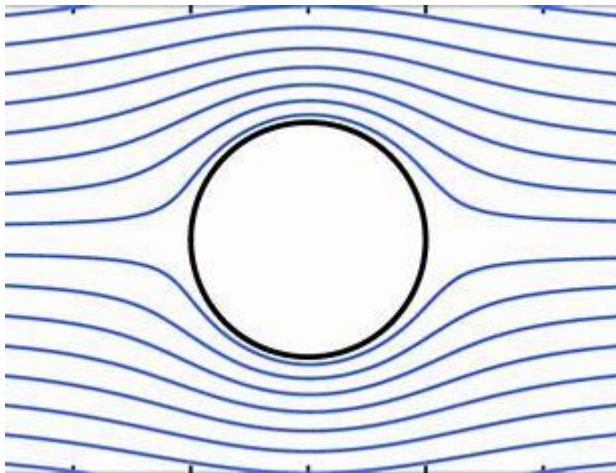
Depending on the **nature of physics** governing the fluid motion **one or more** terms might be **negligible**.

Presence of each term and their combinations determines the appropriate **solution algorithm** and the **numerical procedure**.

Classification of PDEs

Elliptic

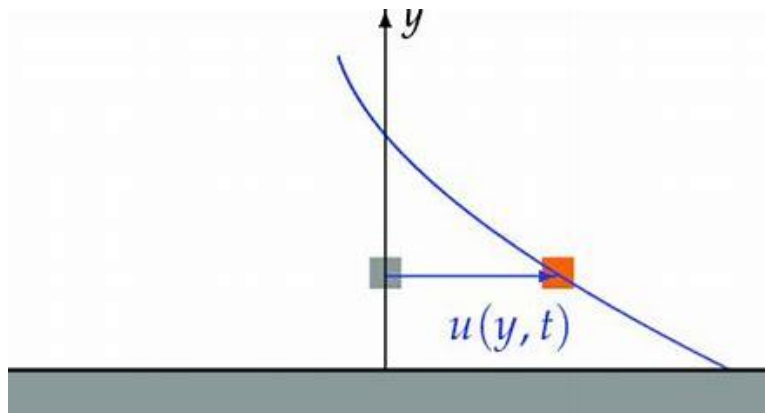
$$\nabla^2 u = 0$$



Potential Flow

Parabolic

$$\frac{\partial u}{\partial t} = \nu \nabla^2 u$$



Flow over an oscillating plate
(Stokes 2nd Problem)

Hyperbolic

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u$$



Wave motion

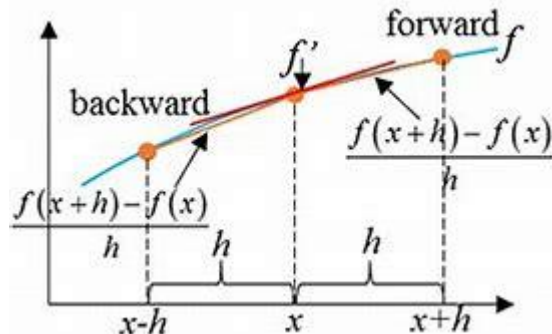
Equations belonging to each of these classifications behave in different ways both *physically* and *numerically*.

Techniques for Numerical Discretization



Commonly used discretization methods

Finite Difference Methods



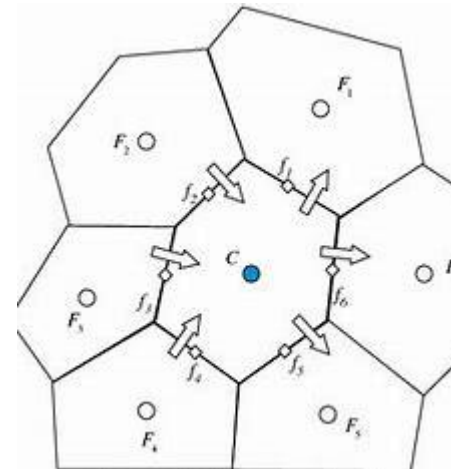
Spectral Methods

$$G(f) = \Im\{\cos(2\pi A t)\} = \int_{-\infty}^{\infty} \frac{e^{i2\pi A t} + e^{-i2\pi A t}}{2} e^{-i2\pi f t} dt$$

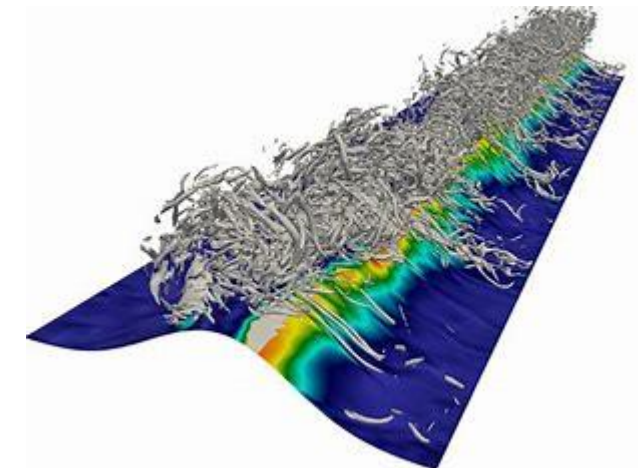
$$= \frac{1}{2} \left[\int_{-\infty}^{\infty} e^{i2\pi A t} e^{-i2\pi f t} dt + \int_{-\infty}^{\infty} e^{-i2\pi A t} e^{-i2\pi f t} dt \right]$$

$$= \frac{1}{2} [\delta(f - A) + \delta(f + A)]$$

Finite Volume Methods



Finite/Spectral Element Methods



Techniques for Numerical Discretization

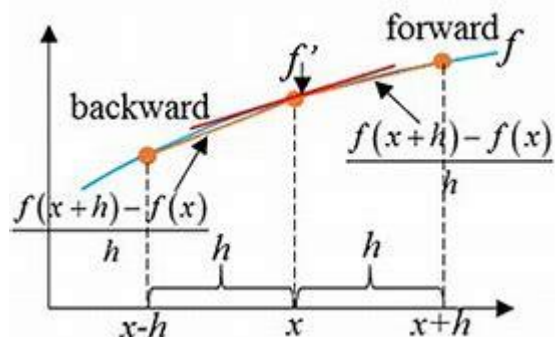
Governing Equations $\xrightarrow{\text{Discretization}}$ Numerical Analogue

Commonly used discretization methods

TODAY

TOMORROW

Finite Difference Methods



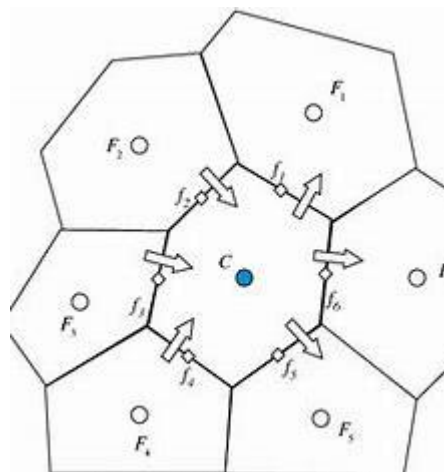
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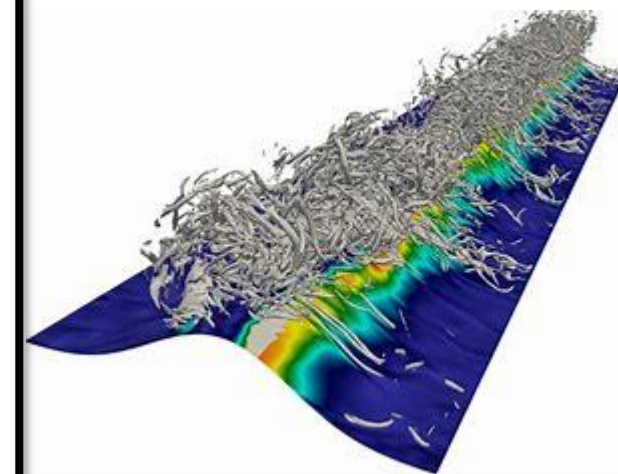
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Finite Volume Methods



Finite/Spectral Element Methods



Finite Difference Method

Definition of a derivative

Exact

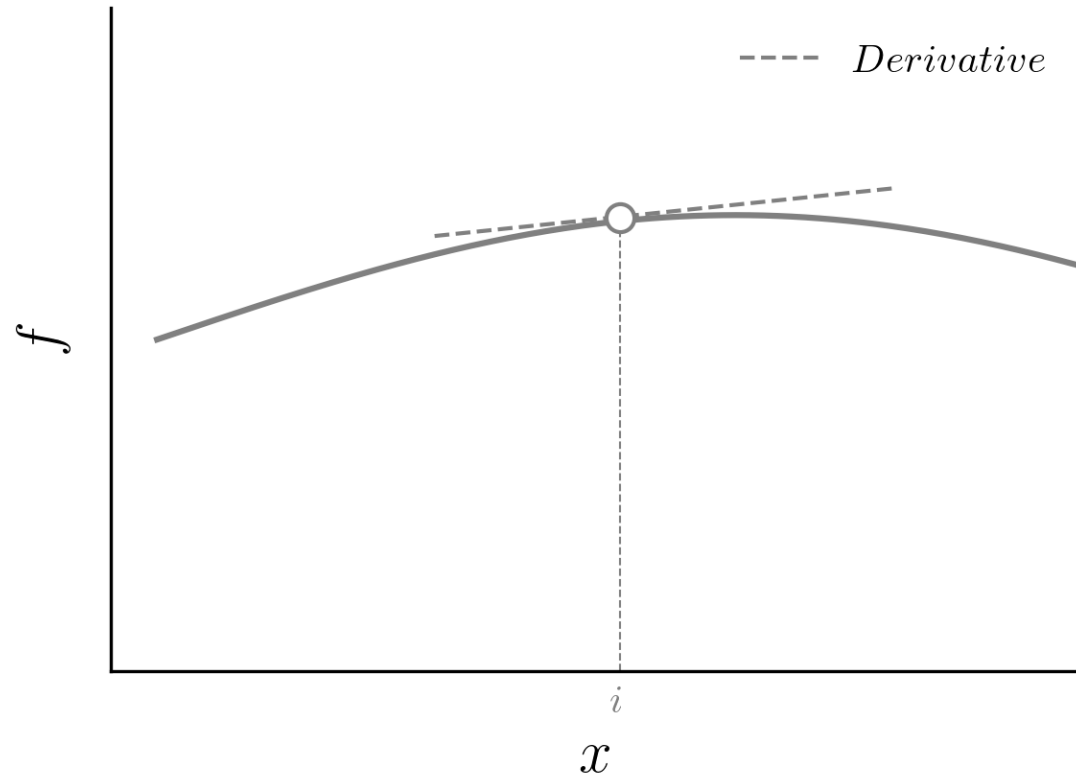
$$\frac{df}{dx} = \lim_{dx \rightarrow 0} \frac{f(x + dx) - f(x)}{dx}$$

Finite Difference Method

Definition of a derivative

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Finite Difference Method

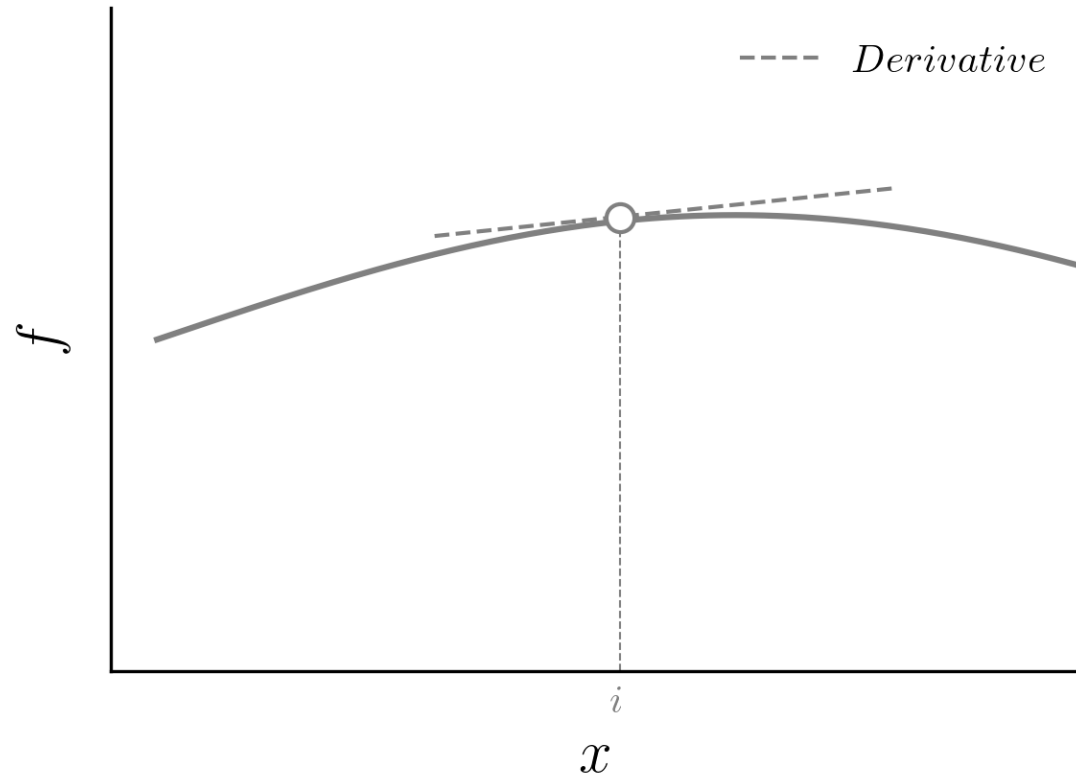
Definition of a derivative

Exact

$$\frac{df}{dx} = \lim_{dx \rightarrow 0} \frac{f(x + dx) - f(x)}{dx}$$

$$\frac{df}{dx} = \lim_{dx \rightarrow 0} \frac{f(x) - f(x - dx)}{dx}$$

$$\frac{df}{dx} = \lim_{dx \rightarrow 0} \frac{f(x + dx) - f(x - dx)}{2dx}$$



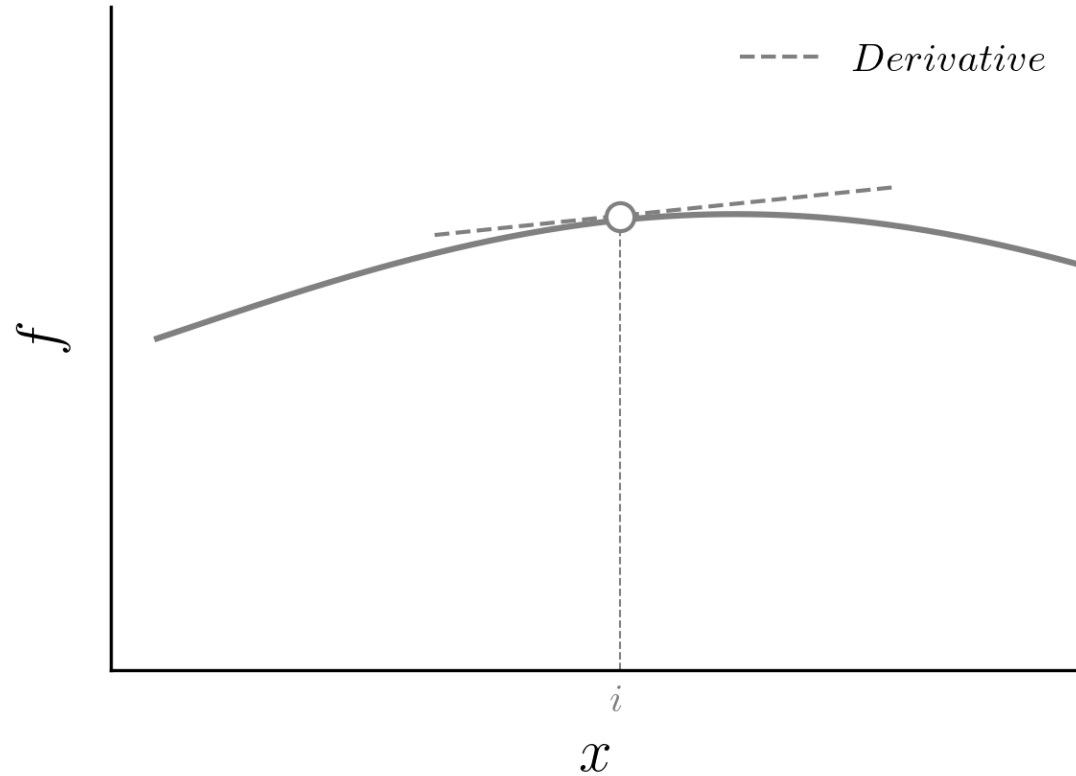
Finite Difference Method

Finite Difference

$$\frac{df}{dx} \approx \frac{f(x + dx) - f(x)}{dx}$$

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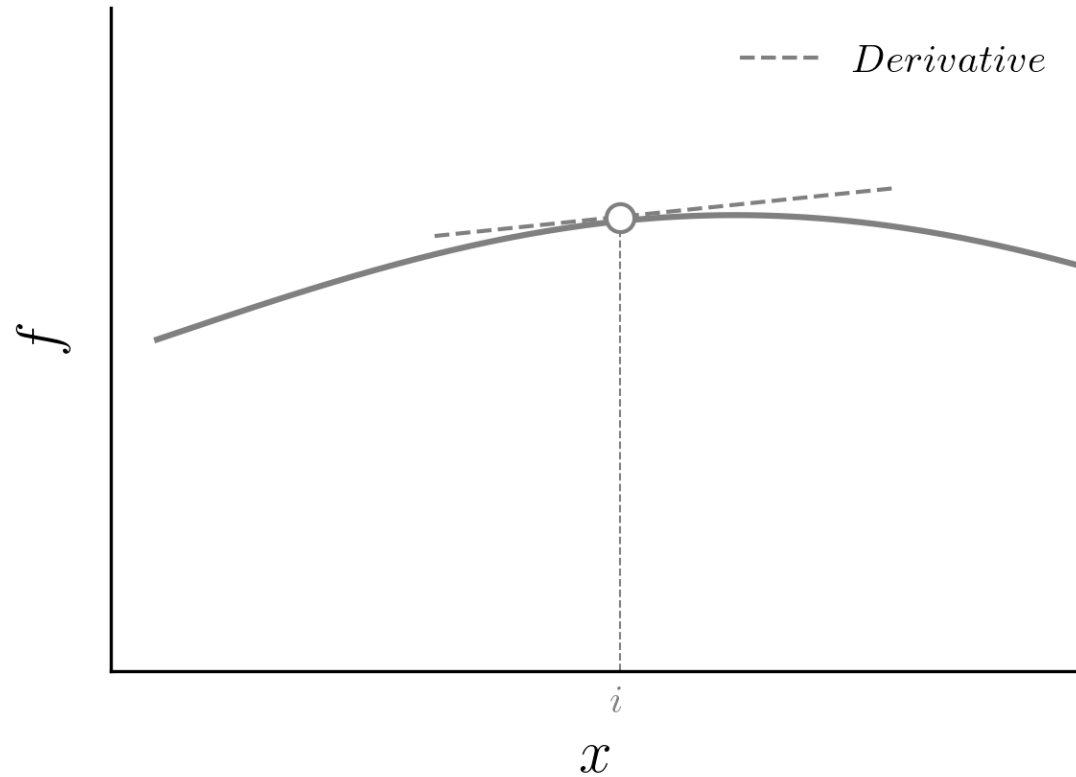
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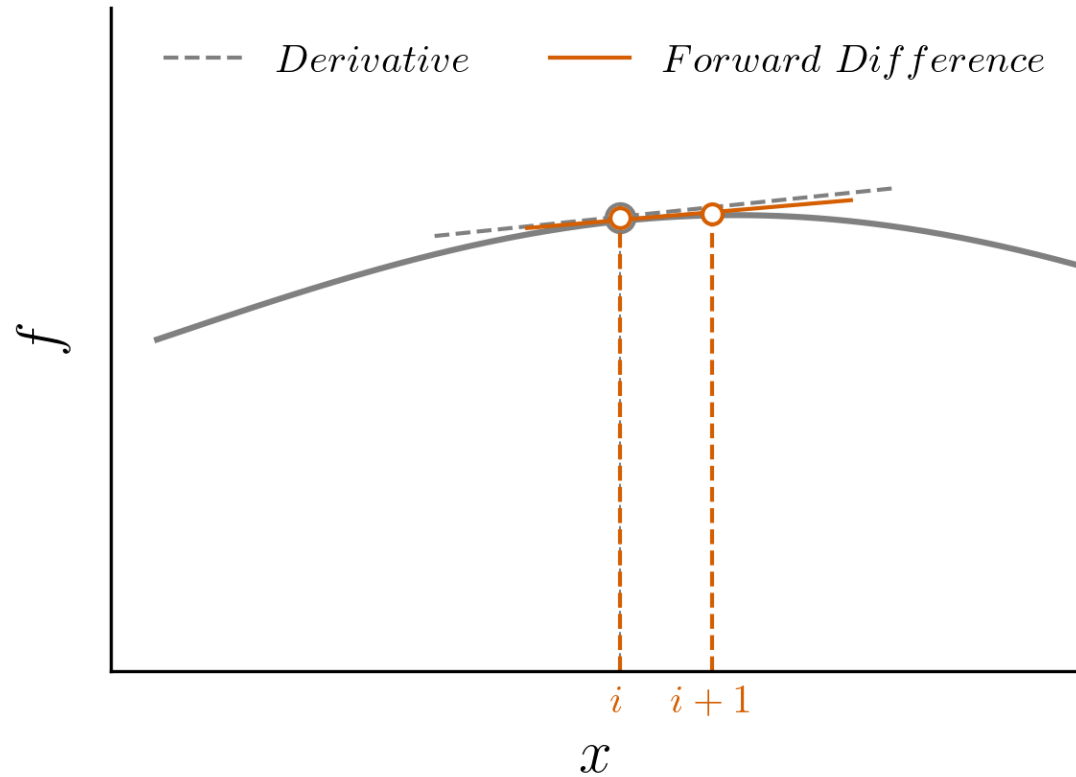


Finite Difference Method

Finite Difference

Forward

$$\frac{df}{dx} \approx \frac{f(x + dx) - f(x)}{dx}$$

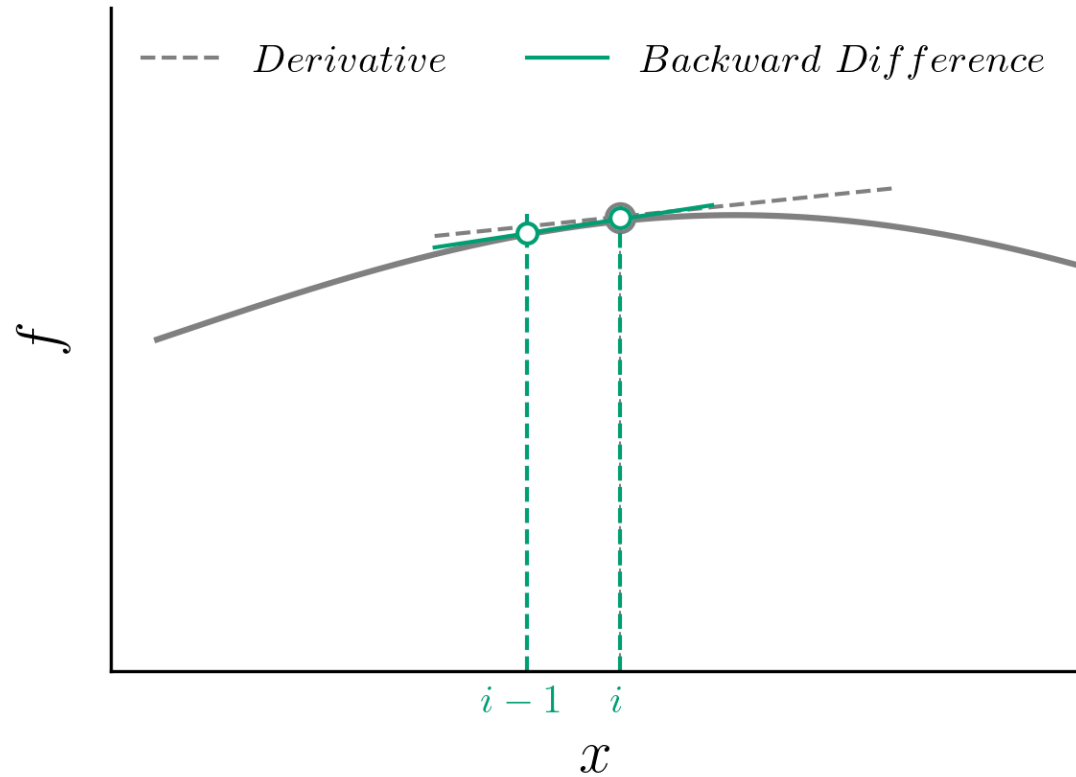


Finite Difference Method

Finite Difference

Forward $\frac{df}{dx} \approx \frac{f(x + dx) - f(x)}{dx}$

Backward $\frac{df}{dx} \approx \frac{f(x) - f(x - dx)}{dx}$



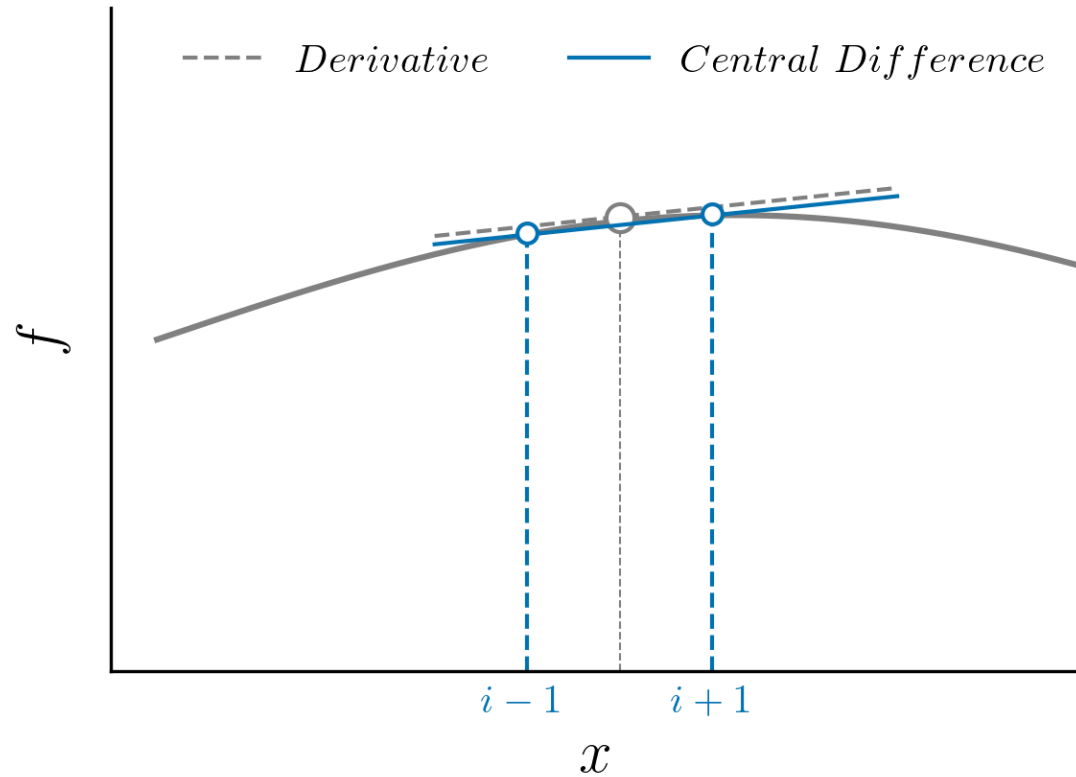
Finite Difference Method

Finite Difference

Forward $\frac{df}{dx} \approx \frac{f(x + dx) - f(x)}{dx}$

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Centered $\frac{df}{dx} \approx \frac{f(x + dx) - f(x - dx)}{2dx}$



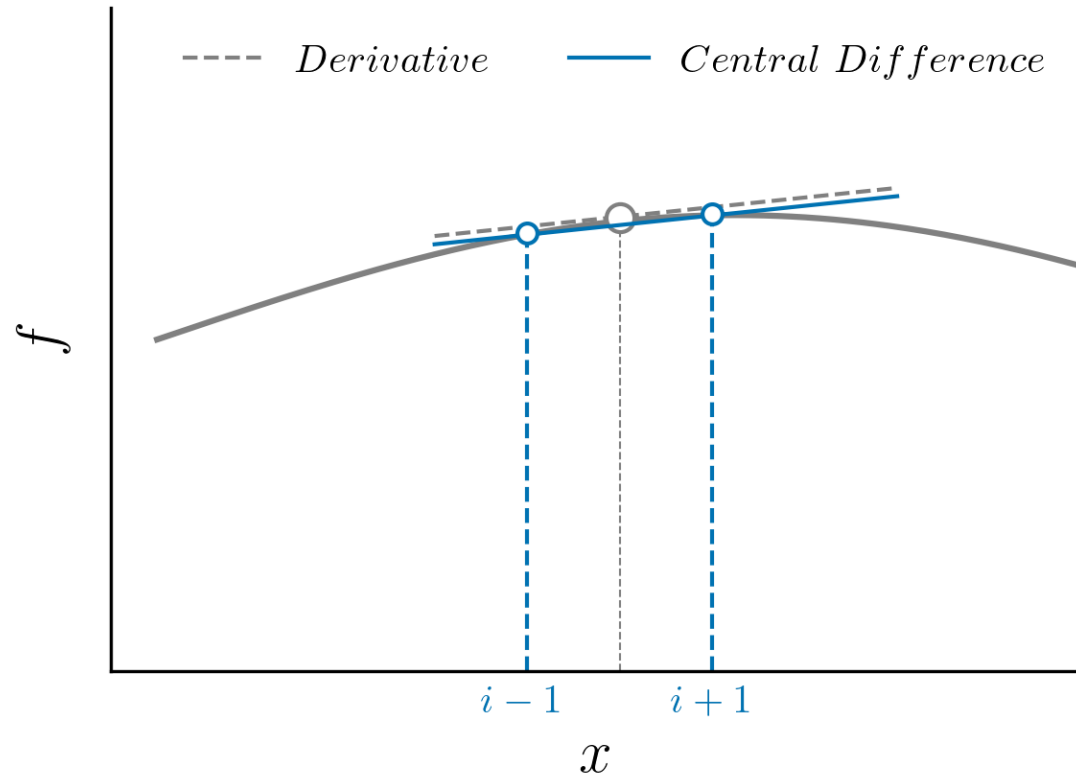
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How good is the approximation?

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Taylor Series

$$f(x_0 + dx) = f(x_0) + \left. \frac{df}{dx} \right|_{x_0} dx + \frac{1}{2!} \left. \frac{d^2 f}{dx^2} \right|_{x_0} dx^2 + \frac{1}{3!} \left. \frac{d^3 f}{dx^3} \right|_{x_0} dx^3 + \dots$$

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$$\frac{f(x_0 + dx) - f(x_0)}{dx} = \frac{df}{dx} \Big|_{x_0} + O(dx)$$

How good is the approximation?

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Taylor Series

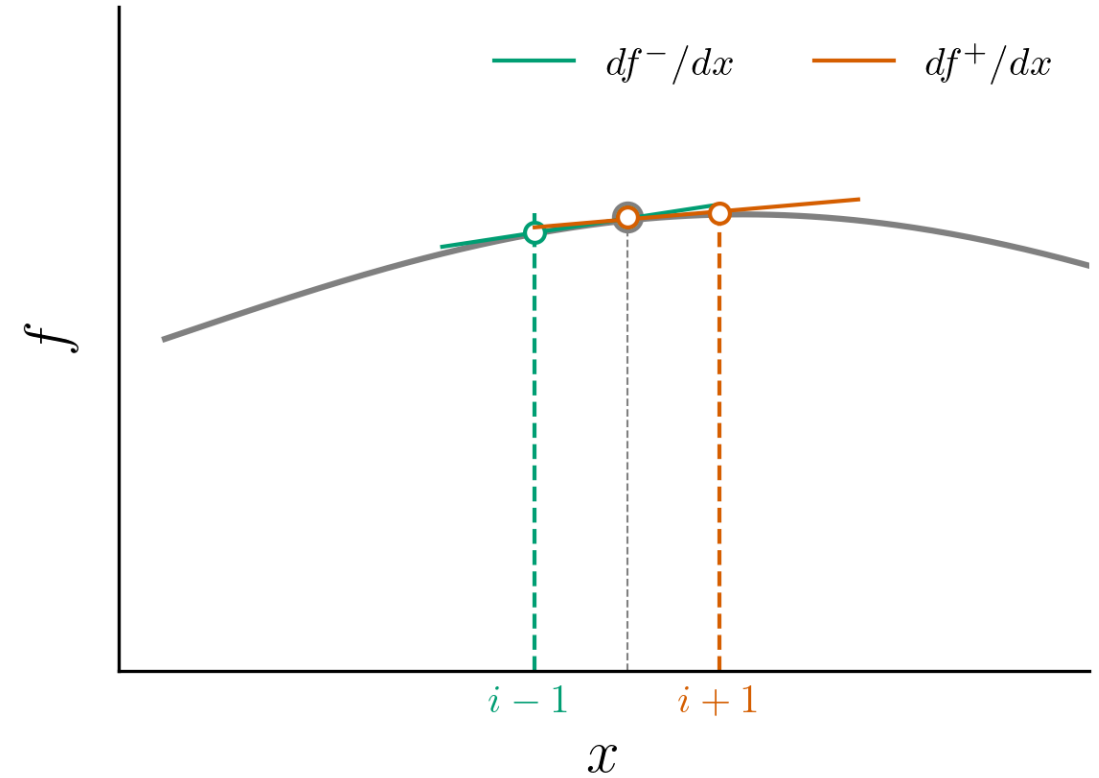
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$$\frac{f(x_0 + dx) - f(x_0)}{dx} = \left. \frac{df}{dx} \right|_{x_0} + O(dx) \longleftarrow 1^{\text{st}} \text{ order accurate}$$

Second derivative

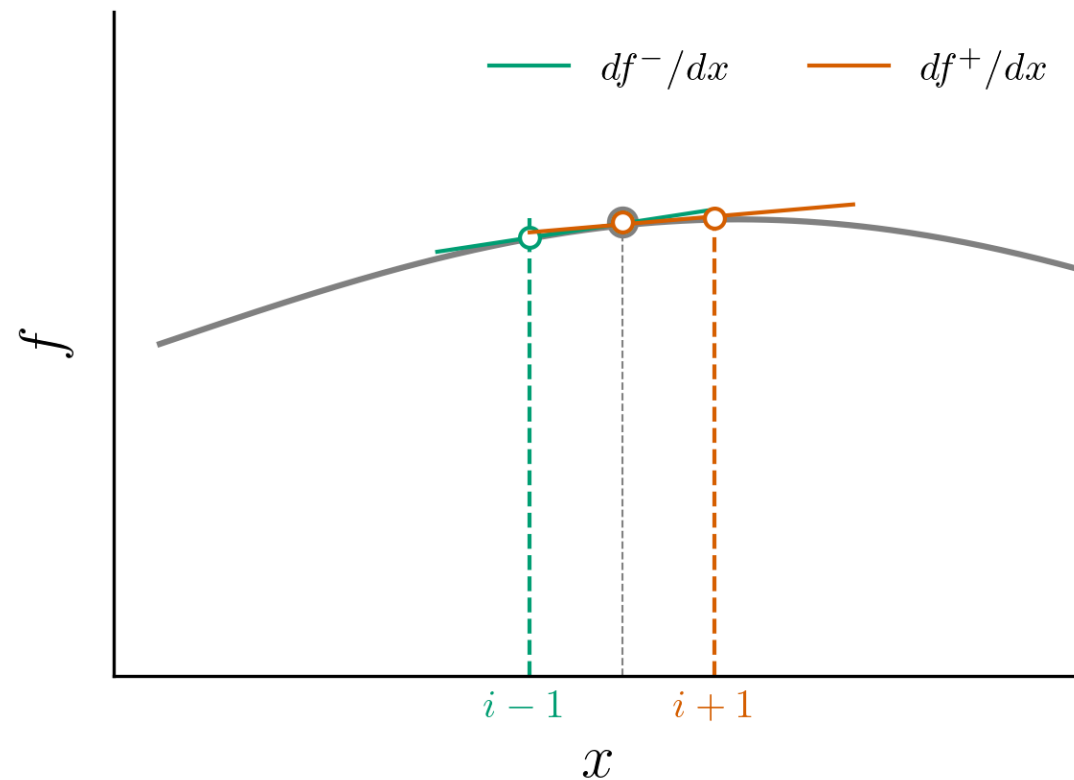
$$\frac{\left. \frac{df}{dx} \right|^+ - \left. \frac{df}{dx} \right|^-}{dx} \approx \frac{d^2 f}{dx^2}$$



Second derivative

$$\frac{\left. \frac{df}{dx} \right|^+ - \left. \frac{df}{dx} \right|^-}{dx} \approx \frac{d^2 f}{dx^2}$$

$$\frac{\frac{f(x+dx) - f(x)}{dx} - \frac{f(x+dx) - f(x)}{dx}}{dx} \approx \frac{d^2 f}{dx^2}$$

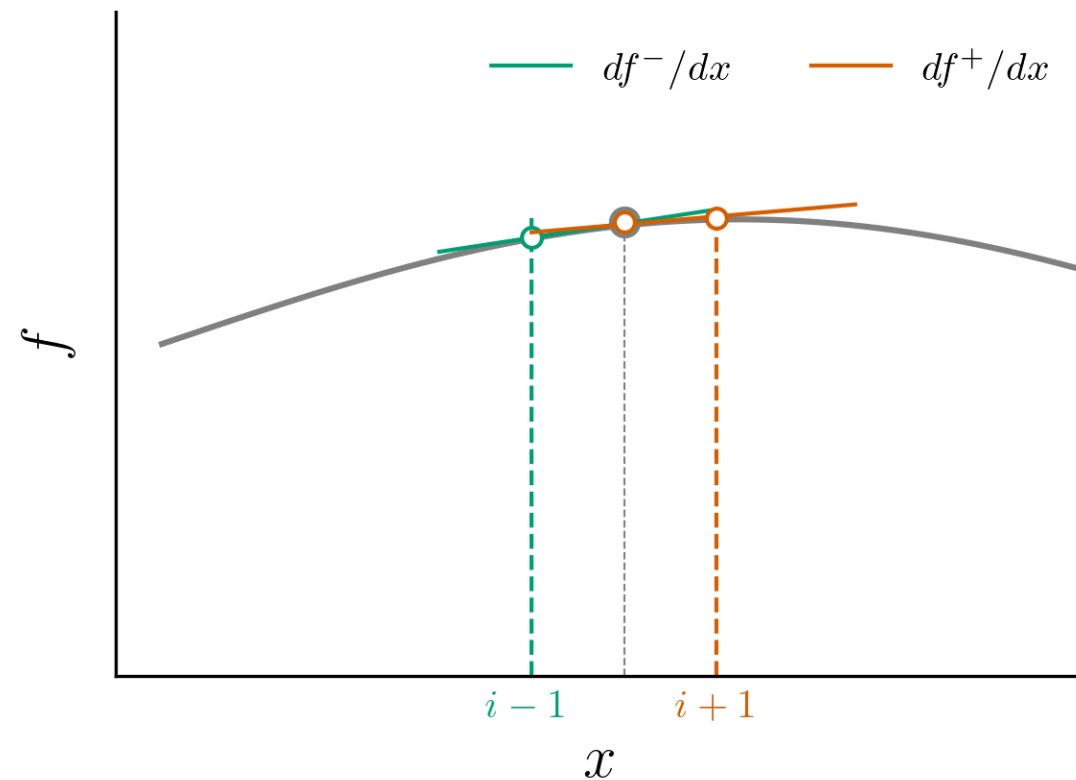


Second derivative

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$$\frac{\frac{f(x+dx) - f(x)}{dx} - \frac{f(x) - f(x-dx)}{dx}}{dx} \approx \frac{d^2 f}{dx^2}$$

$$\frac{f(x+dx) - 2f(x) + f(x-dx)}{dx^2} \approx \frac{d^2 f}{dx^2}$$

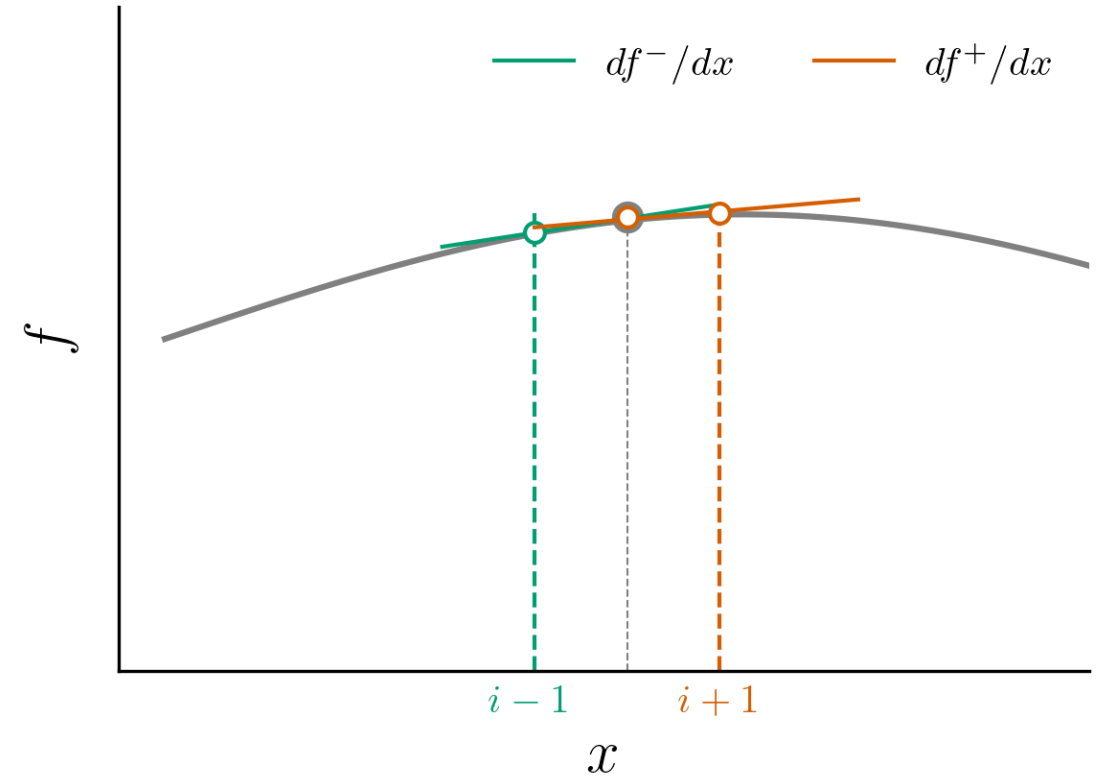


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$$\frac{f(x+dx) - 2f(x) + f(x-dx)}{dx^2} \approx \frac{d^2 f}{dx^2}$$



Central Differencing formula for 2nd derivative

Taylor Series

$$[f(x + dx)] = \left[f(x) + f'(x)dx + \frac{1}{2!}f''(x)dx^2 + \dots \right]$$

$$[f(x)] = [f(x)]$$

$$[f(x - dx)] = \left[f(x) - f'(x)dx + \frac{1}{2!}f''(x)dx^2 + \dots \right]$$

Taylor Series

$$a[f(x + dx)] = a \left[f(x) + f'(x)dx + \frac{1}{2!} f''(x)dx^2 + \dots \right]$$

$$b[f(x)] = b[f(x)]$$

$$c[f(x - dx)] = c \left[f(x) - f'(x)dx + \frac{1}{2!} f''(x)dx^2 + \dots \right]$$

Taylor Series

$$a[f(x + dx)] = a \left[f(x) + f'(x)dx + \frac{1}{2!} f''(x)dx^2 + \dots \right]$$

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$$af(x + dx) + bf(x) + cf(x - dx) \approx (a + b + c)f(x) + (a - c)f'(x)dx + \frac{(a + c)}{2} f''(x)dx^2$$

Derivative Operators

$$af(x + dx) + bf(x) + cf(x - dx) \approx (a + b + c)f(x) + (a - c)f'(x)dx + \frac{(a + c)}{2}f''(x)dx^2$$

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$$a = \frac{1}{2dx}$$

$$b = 0$$

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$$a = \frac{1}{2dx}$$

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2nd Derivative

$$(a + b + c) = 0$$

$$(a - c) = 0$$

$$(a + c) = 2!/dx^2$$

$$\begin{matrix} & A & & w & & S \\ \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & 0 & 1 \end{bmatrix} & \begin{pmatrix} a \\ b \\ c \end{pmatrix} & = & \begin{pmatrix} 0 \\ 0 \\ 2/dx^2 \end{pmatrix} & \xrightarrow{\text{Inversion}} & \end{matrix}$$

$$a = \frac{1}{dx^2}$$

$$b = \frac{-2}{dx^2}$$

$$c = \frac{1}{dx^2}$$

Finite Difference in action

1D Linear Convection

$$\frac{du}{dt} + c \frac{du}{dx} = 0$$

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

Exact Solution:

$$u(x, t) = u_0(x - ct)$$

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$$\frac{du}{dt} + c \frac{du}{dx} = 0$$

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$$\frac{du}{dx} \approx \frac{u(x) - u(x - \Delta x)}{\Delta x}$$

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$$\frac{du}{dt} \approx \frac{u^{n+1}(x) - u^n(x)}{\Delta t}$$

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$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + c \frac{u_i^n - u_{i-1}^n}{\Delta x} = 0$$

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Let's write out 1st CFD code !

1st Code: 1D Linear Convection

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import matplotlib.pyplot as plt
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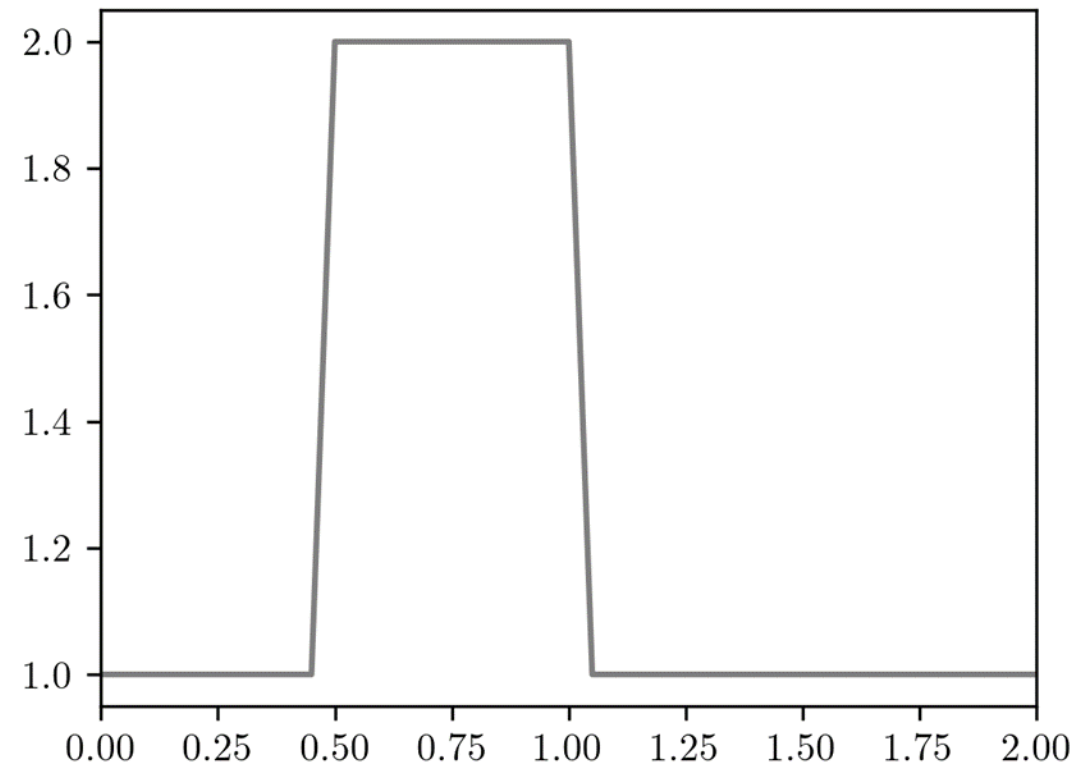
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The initial velocity u_0 is given as 2 in the interval $0.5 \leq x \leq 1$ and 1 elsewhere in $(0,2) \Rightarrow$ Hat function



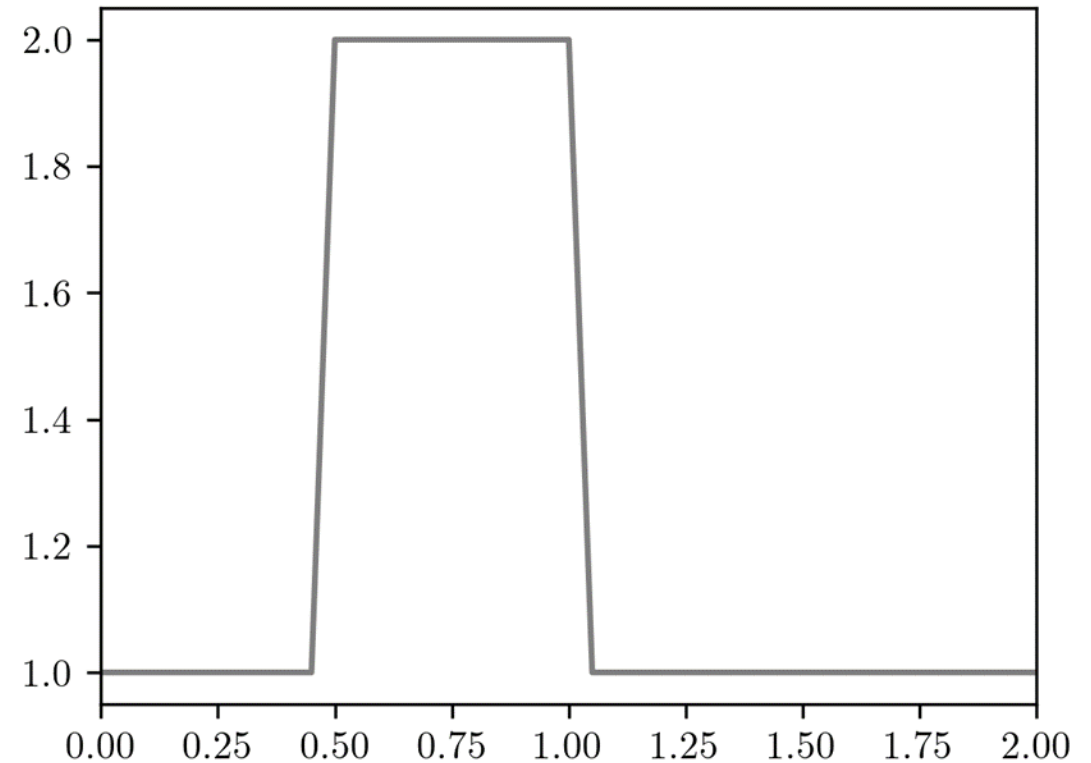
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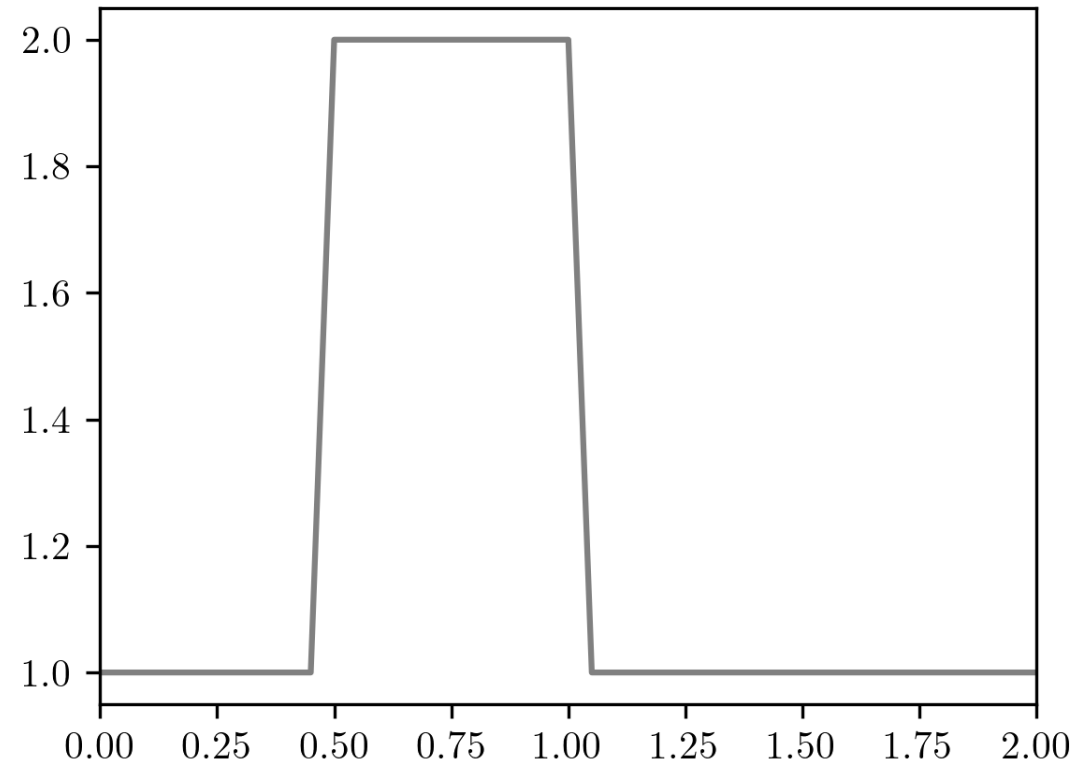
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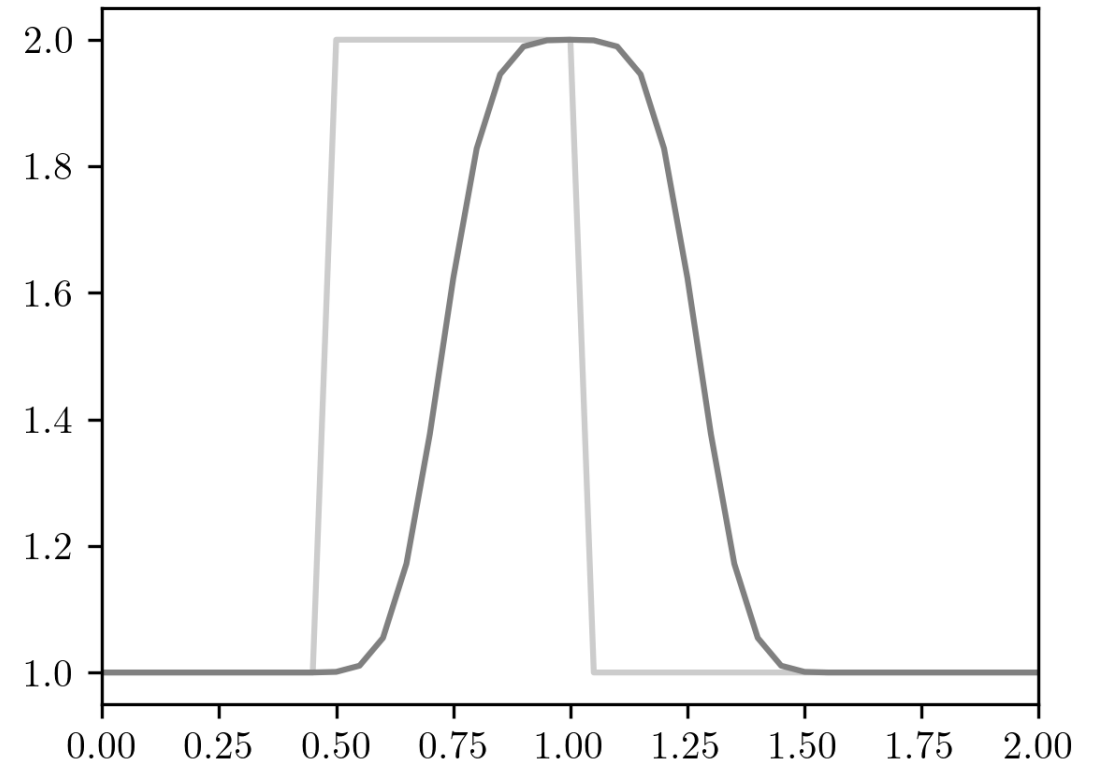
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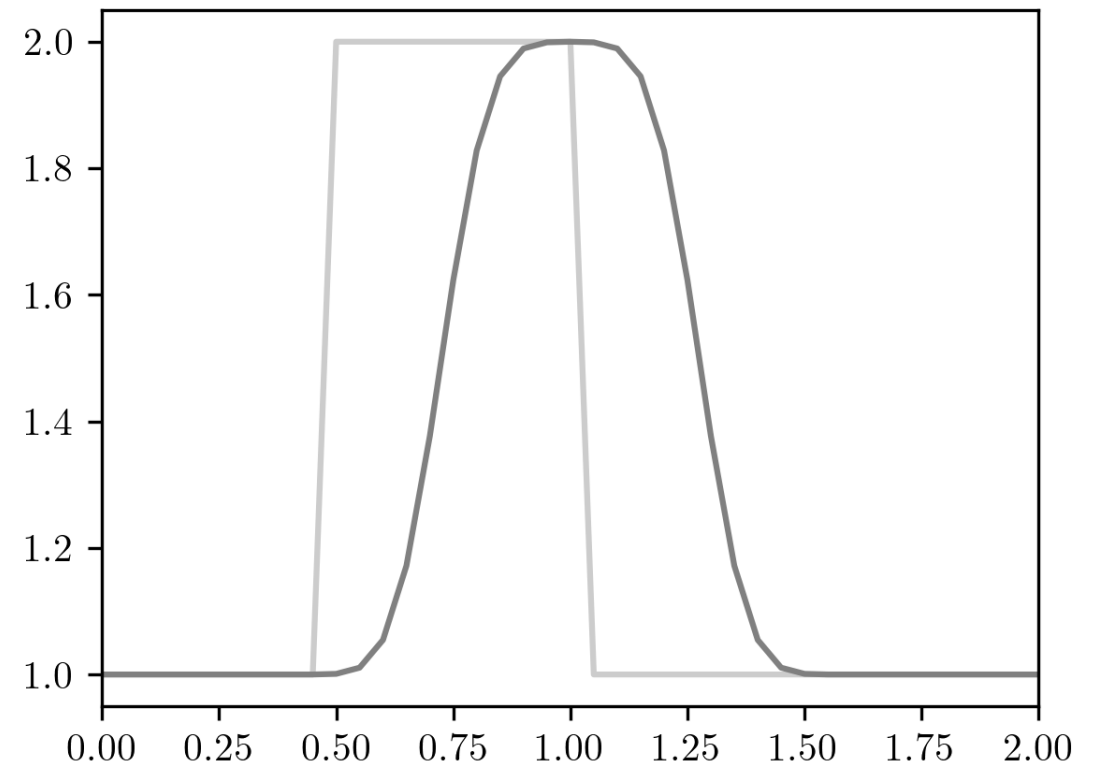
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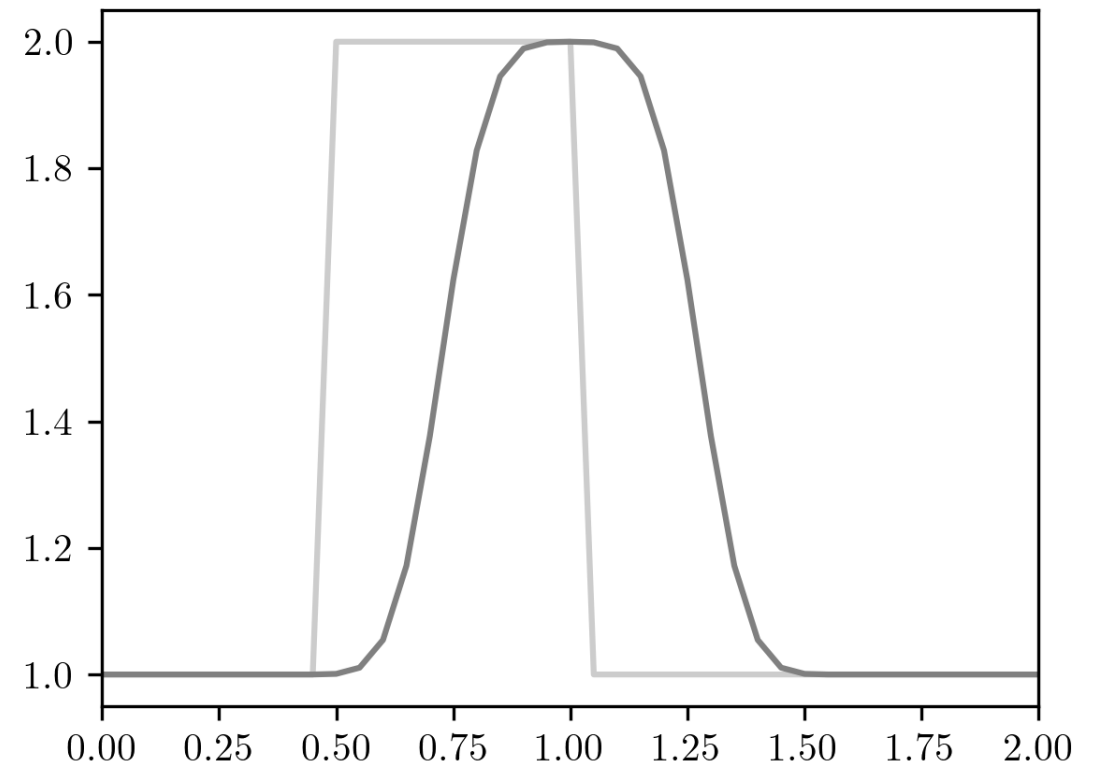
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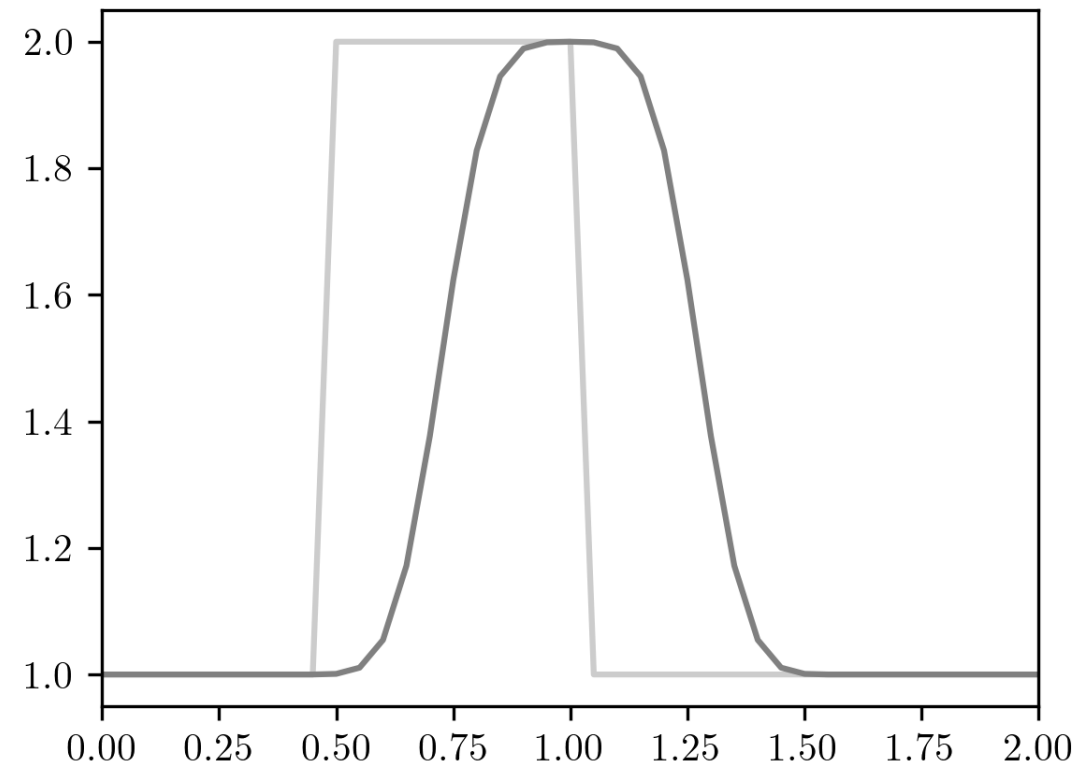
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Change these !

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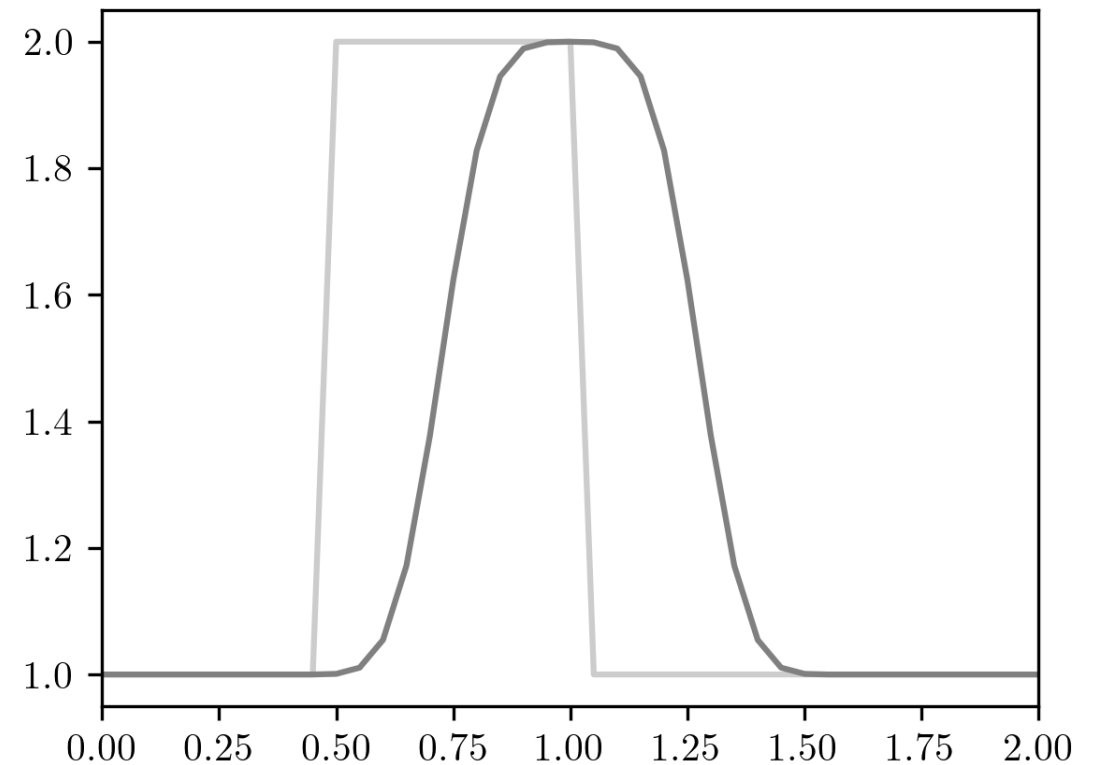
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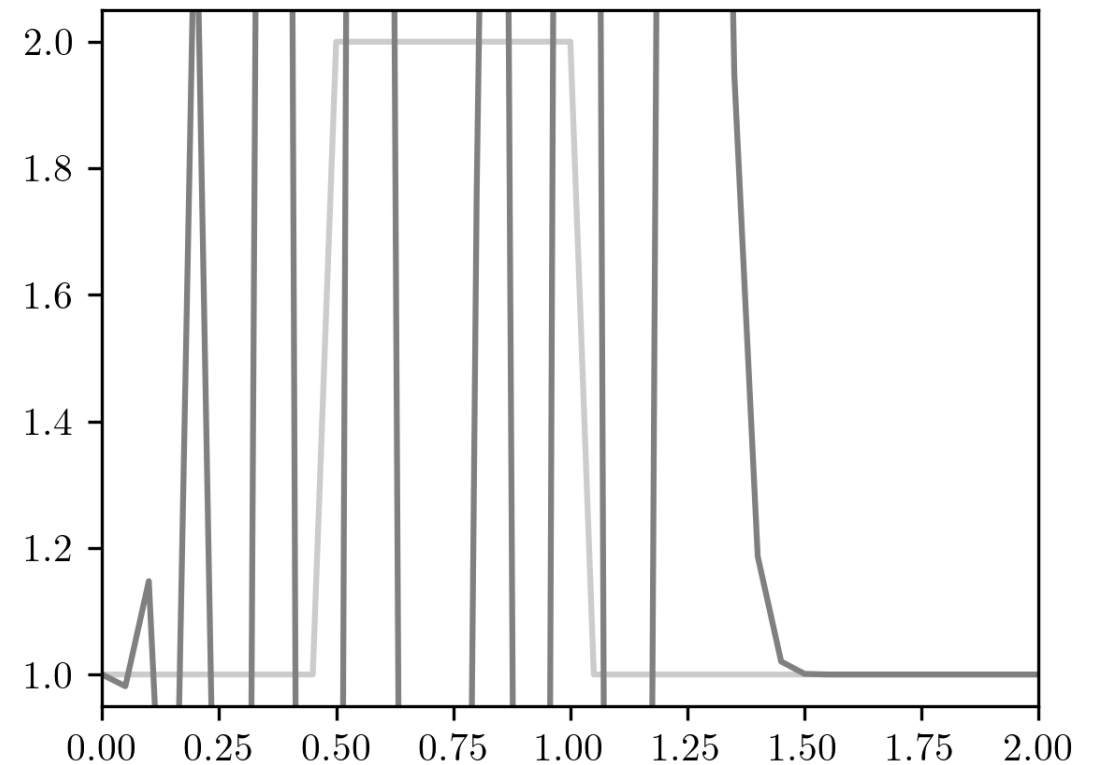
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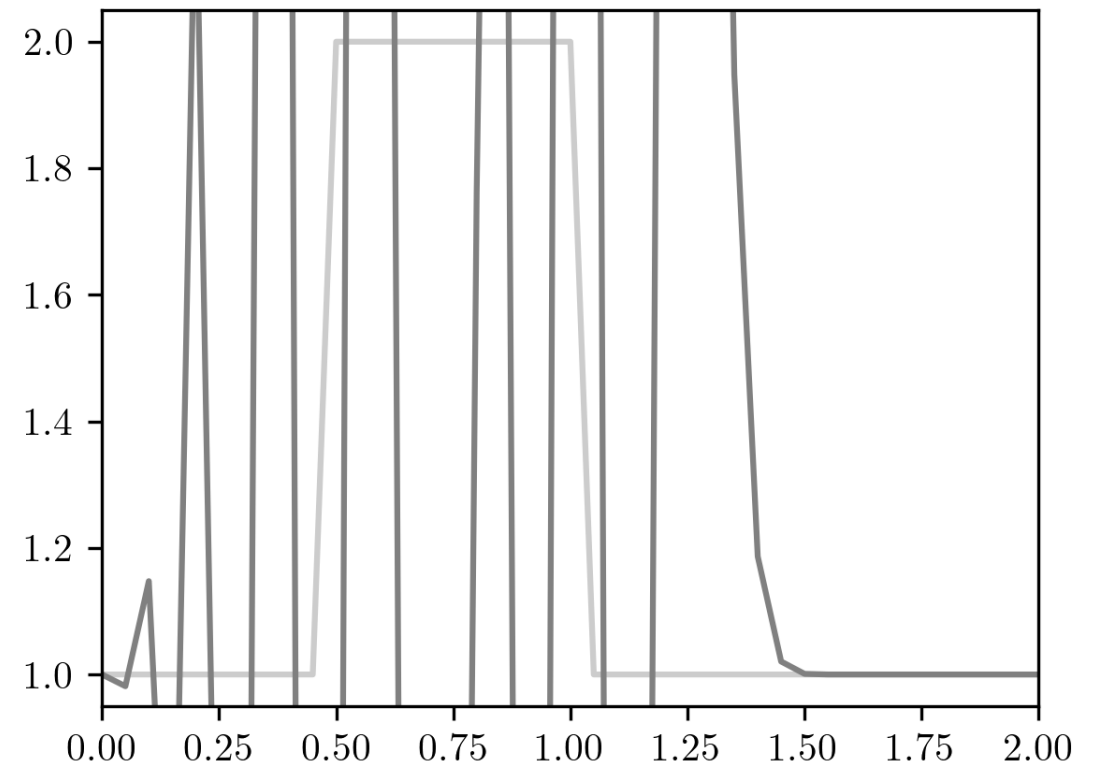
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1D Linear Convection with Central Differencing in Space

$$\frac{du}{dt} + c \frac{du}{dx} = 0 \longrightarrow \frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{c}{2\Delta x} (u_{i+1}^n - u_{i-1}^n) = 0$$

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Truncation Error (ϵ_t)

1D Linear Convection with Central Differencing in Space

$$\frac{du}{dt} + c \frac{du}{dx} = 0 \longrightarrow \frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{c}{2\Delta x} (u_{i+1}^n - u_{i-1}^n) = 0$$

$$u_i^{n+1} = u_i^n + \Delta t \left. \frac{\partial u}{\partial t} \right|_i^n + \frac{\Delta t^2}{2!} \left. \frac{\partial^2 u}{\partial t^2} \right|_i^n + \frac{\Delta t^3}{3!} \left. \frac{\partial^3 u}{\partial t^3} \right|_i^n + \dots$$

$$u_{i+1}^n = u_i^n + \Delta x \left. \frac{\partial u}{\partial x} \right|_i^n + \frac{\Delta x^2}{2!} \left. \frac{\partial^2 u}{\partial x^2} \right|_i^n + \frac{\Delta x^3}{3!} \left. \frac{\partial^3 u}{\partial x^3} \right|_i^n + \dots$$

$$u_{i-1}^n = u_i^n - \Delta x \left. \frac{\partial u}{\partial x} \right|_i^n + \frac{\Delta x^2}{2!} \left. \frac{\partial^2 u}{\partial x^2} \right|_i^n - \frac{\Delta x^3}{3!} \left. \frac{\partial^3 u}{\partial x^3} \right|_i^n + \dots$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{c}{2\Delta x} (u_{i+1}^n - u_{i-1}^n) - \left(\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} \right)_i^n = \frac{\Delta t}{2!} \left. \frac{\partial^2 u}{\partial t^2} \right|_i^n + \frac{c\Delta x^3}{3!} \left. \frac{\partial^3 u}{\partial t^3} \right|_i^n + O(\Delta t^2, \Delta x^4)$$

Truncation Error (ϵ_t)

As Δt & $\Delta x \rightarrow 0$: $\epsilon_T \rightarrow 0 \Rightarrow$ Numerical Scheme is Consistent

1D Linear Convection with Central Differencing in Space

Consider the exact solution of the discretized equation:

$$\frac{\overline{u_i^{n+1}} - \overline{u_i^n}}{\Delta t} + \frac{c}{2\Delta x} (\overline{u_{i+1}^n} - \overline{u_{i-1}^n}) = 0$$

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$$(\overline{u_t})_i^n = -c (\overline{u_x})_i^n + O(\Delta t, \Delta x)$$

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Modified Differential Equation !

$$\overline{(u_{tt})}_i^n = -c \overline{[(u_t)]_{x_i}}_i^n + O(\Delta t, \Delta x)$$

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$$\overline{(u_{tt})}_i^n = -c \overline{[(u_t)]_{x_i}}^n + O(\Delta t, \Delta x)$$

NOT a convection equation, It is a **Convection-Diffusion** equation !!

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-ve Diffusion Coefficient !!

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Explosion : Unstable Scheme !!

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Diffusion Coefficient must be +ve !!

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For stability, we need: $0 \leq \frac{c\Delta t}{\Delta x} \leq 1$

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↑
Courant-Friedrich-Lewy (CFL) Number!!

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For a CFL of < 1: Numerical Diffusion is of $O(\Delta x)$

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For a CFL of < 1: Numerical Diffusion is of $O(\Delta x)$

Poor Accuracy !!

2nd Code: 1D non-Linear Convection

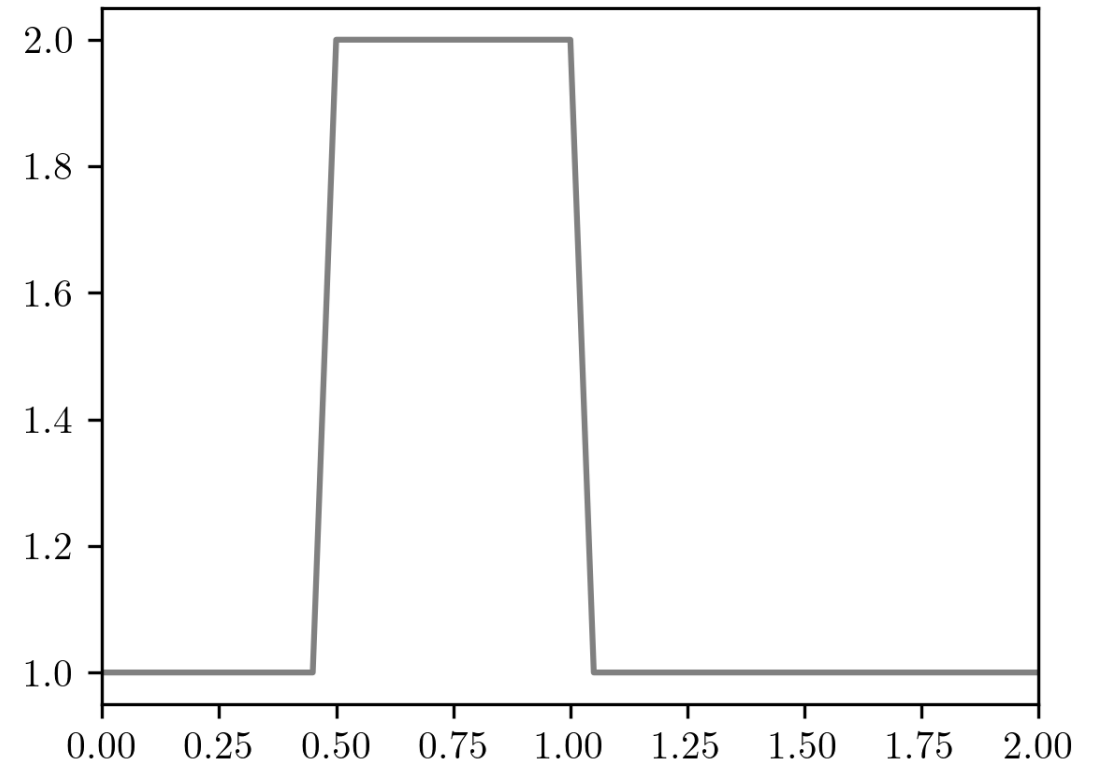
```
import numpy as np
import matplotlib.pyplot as plt
import time, sys

nx = 41
dx = 2/(nx-1)
nt = 25
dt = 0.025
c = 1

u = np.ones(nx)
u[int(0.5/dx):int(1/dx+1)] = 2
print(u)
plt.plot(np.linspace(0,2,nx), u)

un = np.ones(nx)
for n in range(nt):
    un=u.copy()
    for i in range(1,nx):
        u[i] = un[i] - c * dt/dx * (un[i]-un[i-1])
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```

The initial velocity u_0 is given as 2 in the interval $0.5 \leq x \leq 1$ and 1 elsewhere in $(0,2) \Rightarrow$ Hat function



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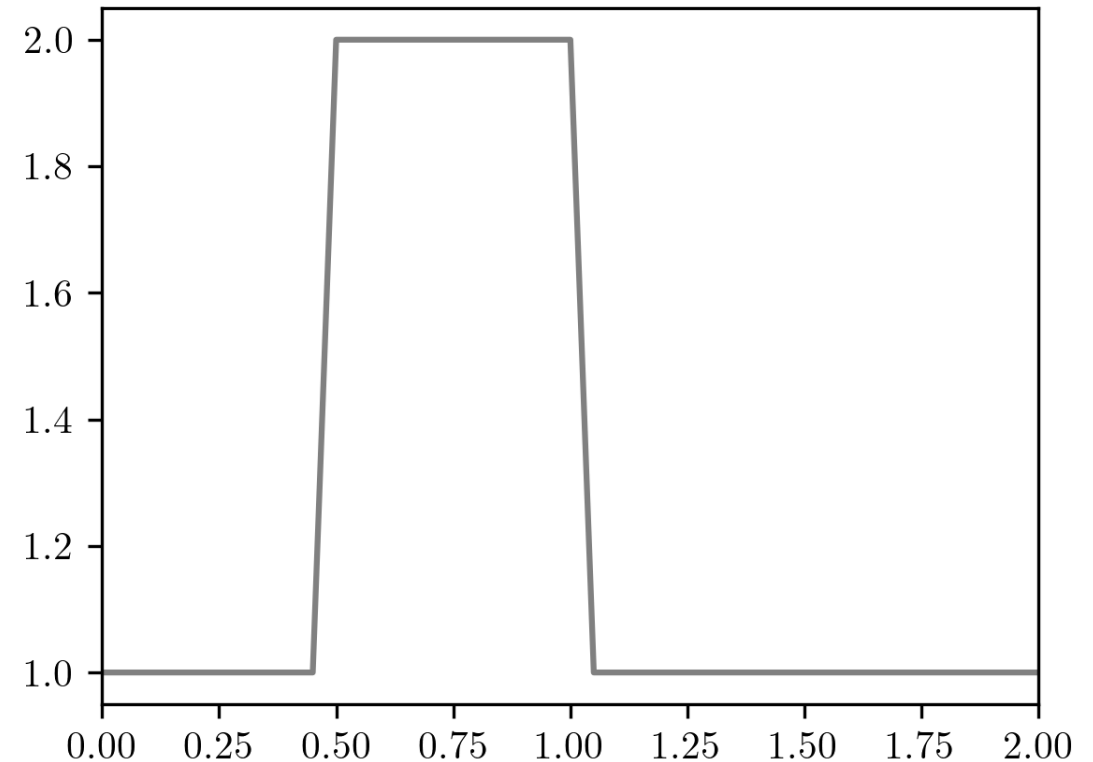
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dx = 2/(nx-1)
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```
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```

```
un = np.ones(nx)
for n in range(nt):
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        u[i] = un[i] - c * dt/dx * (un[i]-un[i-1])
    plt.plot(np.linspace(0,2,nx), u)
```

change this only !

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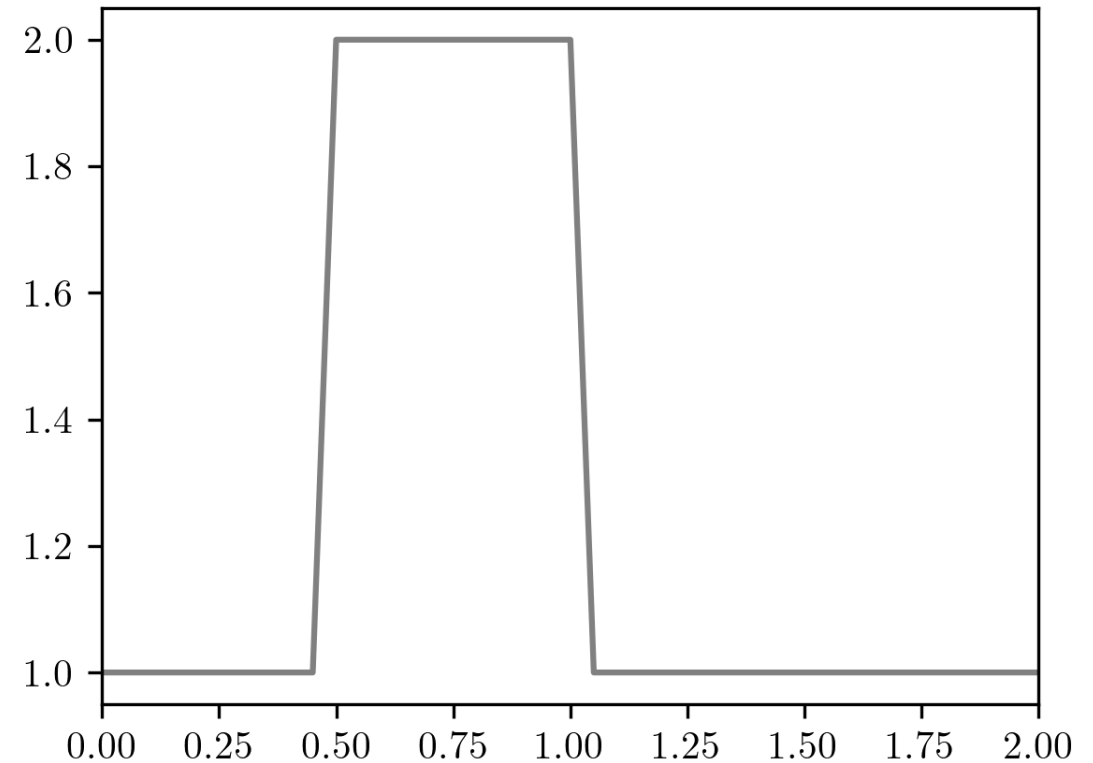
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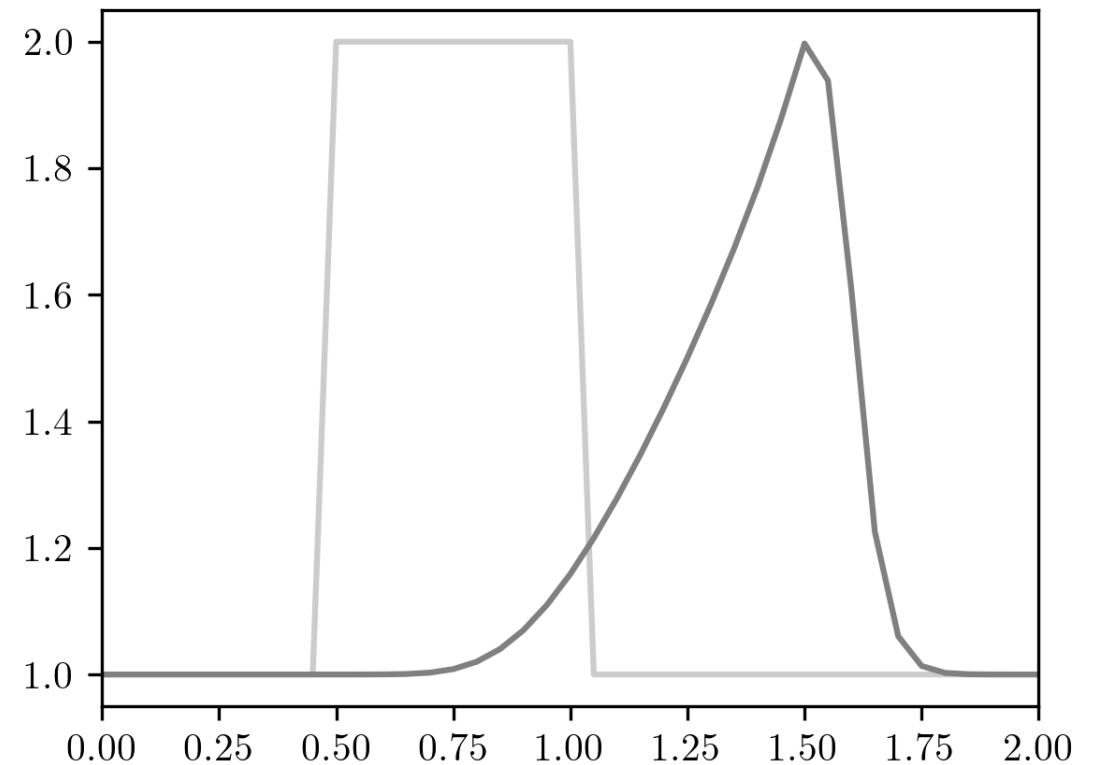
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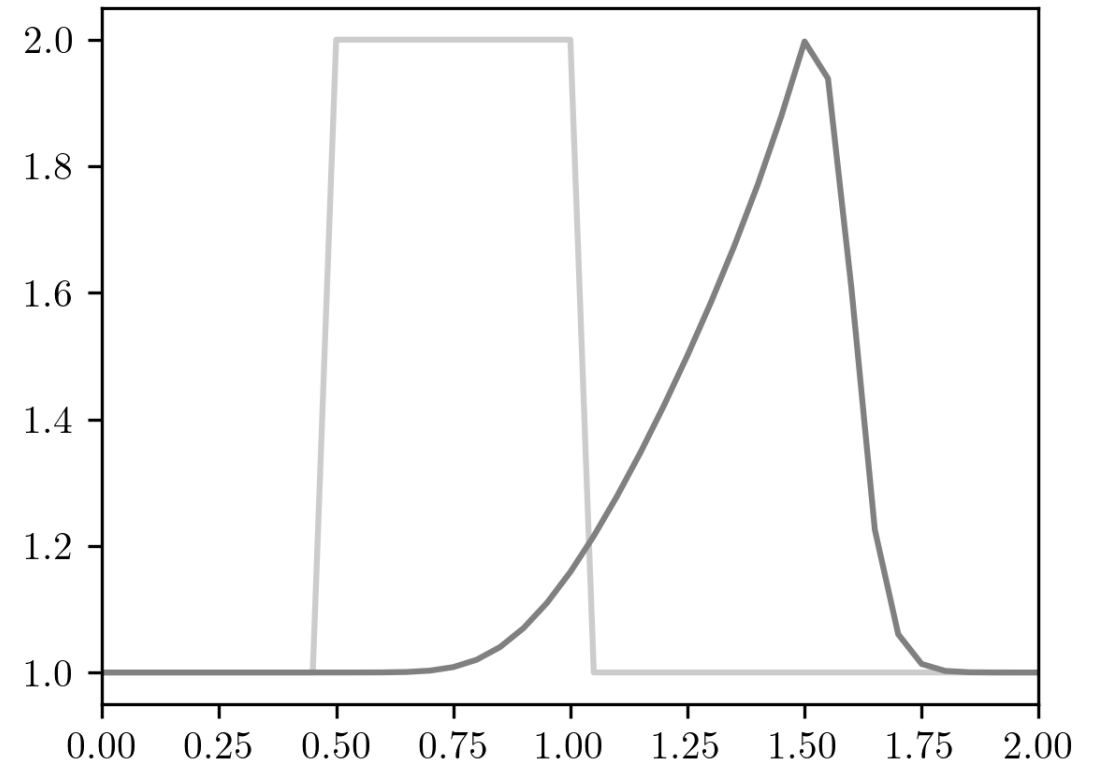
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Let's introduce
CFL

The initial velocity u_0 is given as 2 in the interval $0.5 \leq x \leq 1$ and 1 elsewhere in $(0,2) \Rightarrow$ Hat function



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```
import numpy as np
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```
nx = 41
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CFL = 0.9

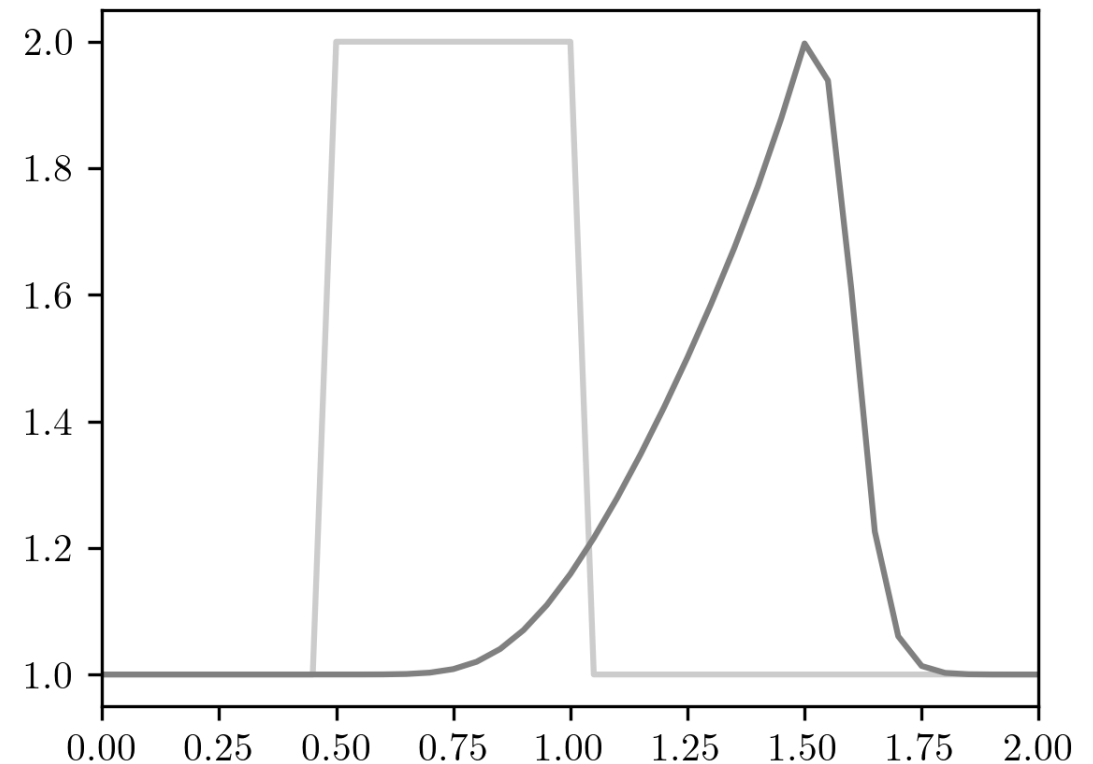
u = np.ones(nx)
u[int(0.5/dx):int(1/dx+1)] = 2
print(u)
plt.plot(np.linspace(0,2,nx), u)

dt = CFL*dx/max(abs(u))

un = np.ones(nx)
for n in range(nt):
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    for i in range(1,nx):
        u[i] = un[i] - un[i] * dt/dx * (un[i]-un[i-1])
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nt = 25
CFL = 0.9

u = np.ones(nx)
u[int(0.5/dx):int(1/dx+1)] = 2
print(u)
plt.plot(np.linspace(0,2,nx), u)
```

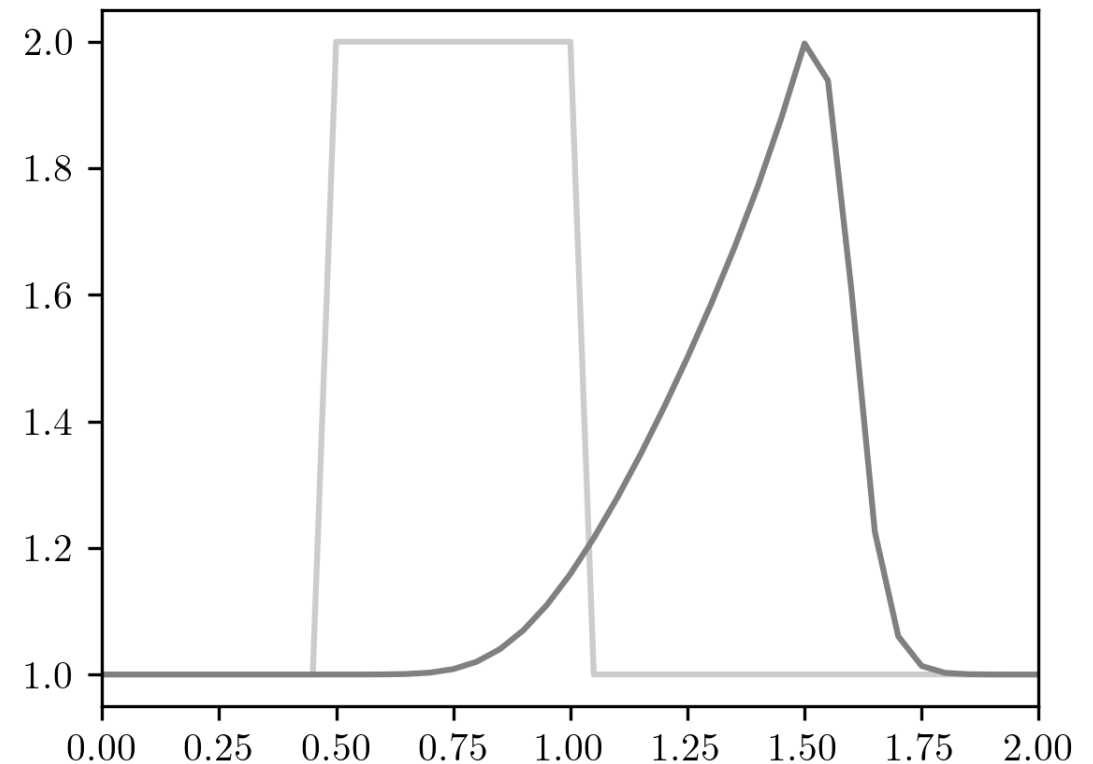
Let's introduce
CFL

```
dt = CFL*dx/max(abs(u))

un = np.ones(nx)
for n in range(nt):
    un=u.copy()
    for i in range(1,nx):
        u[i] = un[i] - un[i] * dt/dx * (un[i]-un[i-1])
plt.plot(np.linspace(0,2,nx), u)
```

Play a bit & see
what happens!

The initial velocity u_0 is given as 2 in the interval $0.5 \leq x \leq 1$ and 1 elsewhere in $(0,2) \Rightarrow$ Hat function



3rd Code: 1D Diffusion

$$\frac{du}{dt} = \nu \frac{d^2u}{dx^2}$$

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Exponential Damping for $v > 0$

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Diffusion is isotropic in nature

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No Directional Bias

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Central-Differencing

3rd Code: 1D Diffusion

$$\frac{du}{dt} = \nu \frac{d^2u}{dx^2}$$

Central Difference

$$\frac{d^2u}{dx^2} \approx \frac{u(x + \Delta x) - 2u(x) + u(x - \Delta x)}{\Delta x^2}$$

Forward Euler

$$\frac{du}{dt} \approx \frac{u^{n+1}(x) - u^n(x)}{\Delta t}$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \nu \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}$$

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Let's Code It !

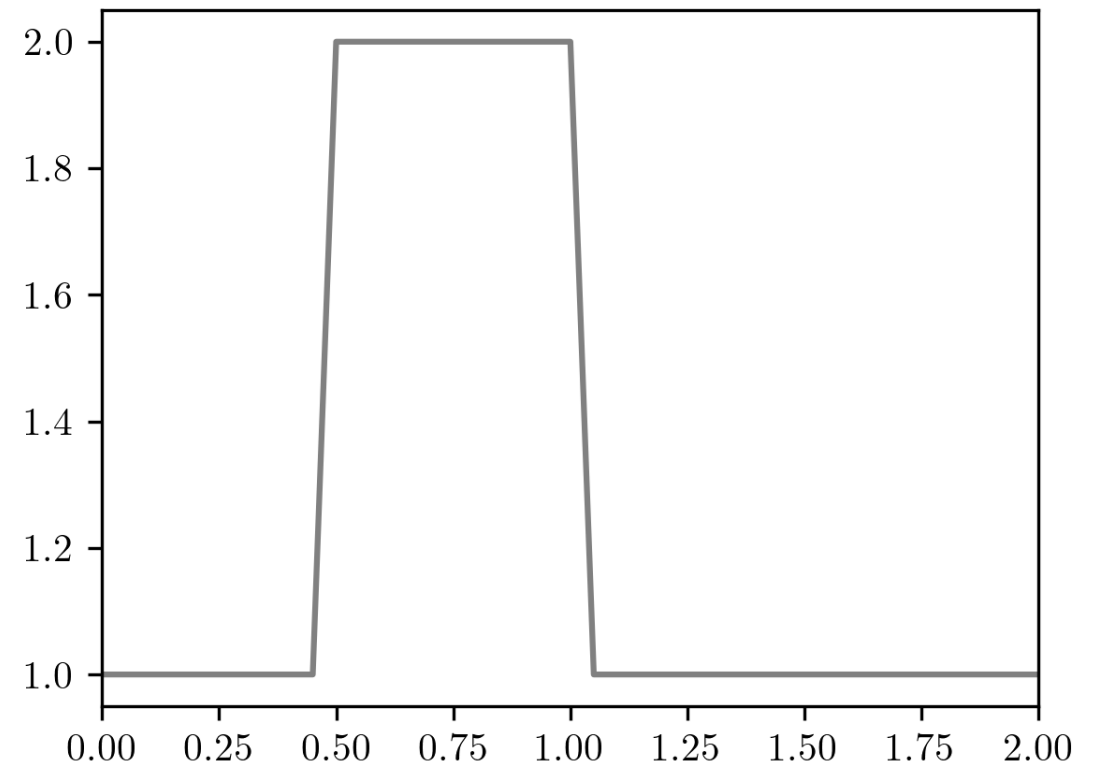
3rd Code: 1D Diffusion

```
import numpy as np
import matplotlib.pyplot as plt
import time, sys
```

```
nx = 41; dx = 2/(nx-1)
nt = 25
nu = 0.3
sigma = 0.2
dt = sigma * dx**2 / nu

u = np.ones(nx)
u[int(0.5/dx):int(1/dx+1)] = 2
print(u)
plt.plot(np.linspace(0,2,nx), u)
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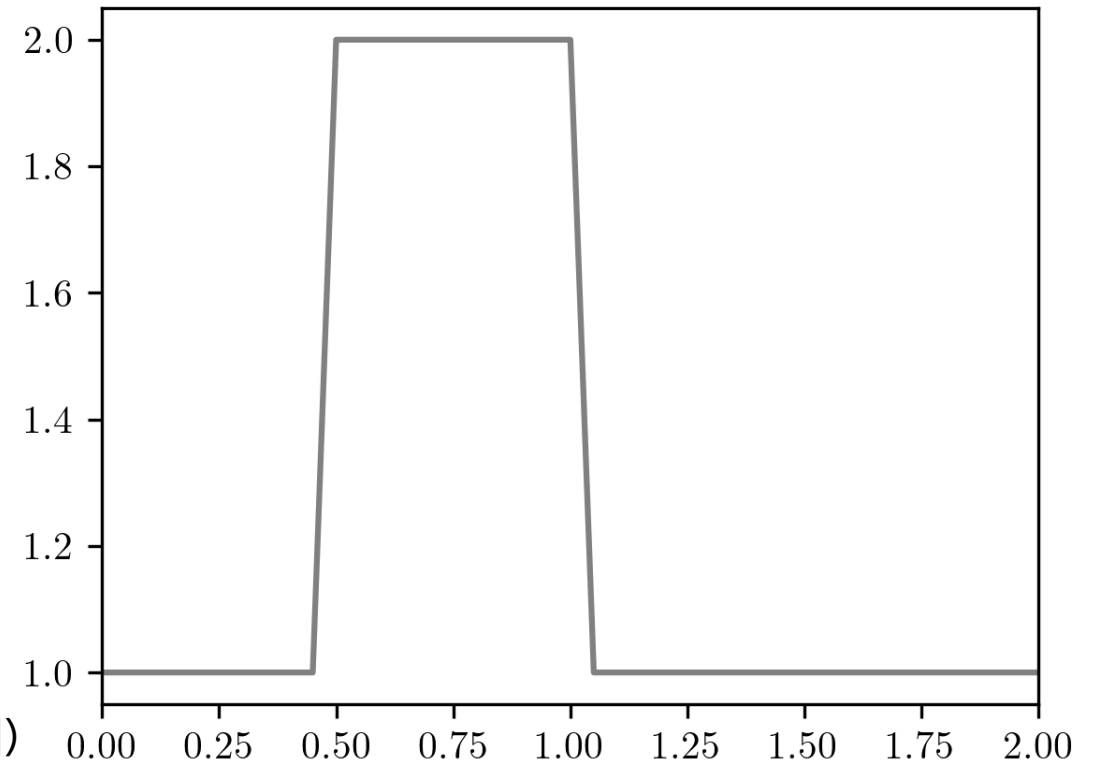
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u[int(0.5/dx):int(1/dx+1)] = 2
print(u)
plt.plot(np.linspace(0,2,nx), u)

un = np.ones(nx)
for n in range(nt):
    un=u.copy()
    for i in range(1,nx-1):
        u[i] = un[i] + nu * dt/dx**2 * (un[i+1]-2*un[i]+un[i-1])
plt.plot(np.linspace(0,2,nx), u)
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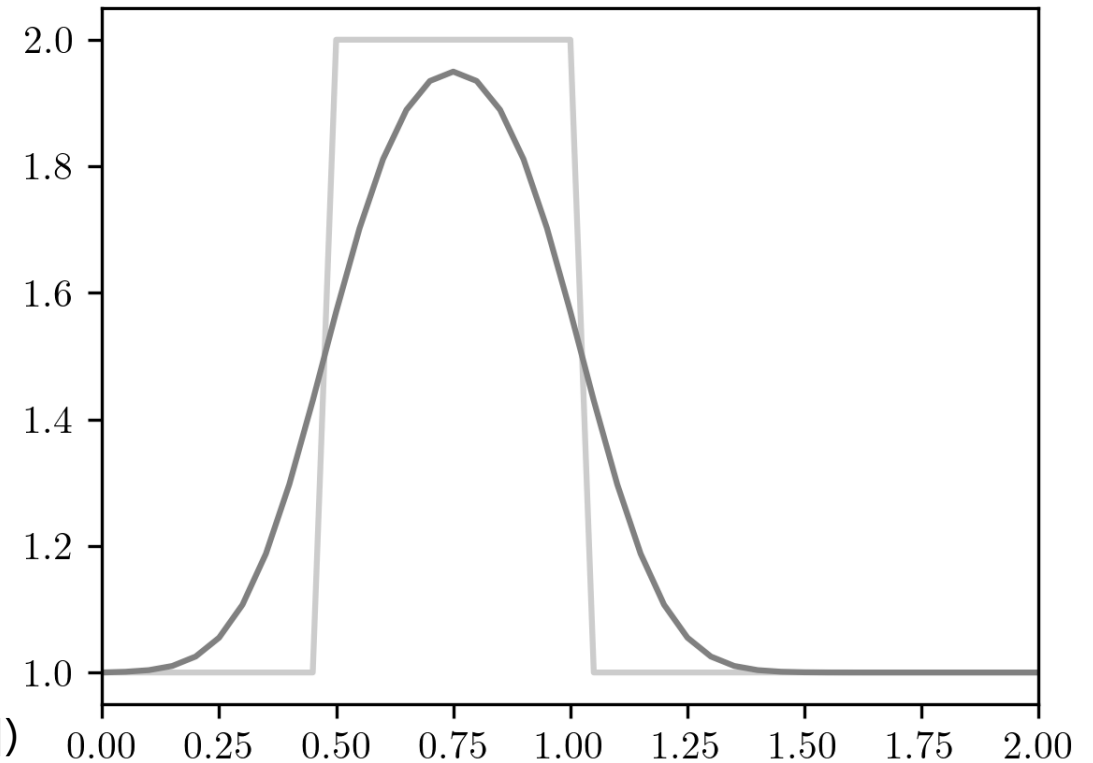
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1D Diffusion (Caution!)

$$\frac{du}{dt} = \nu \frac{d^2u}{dx^2}$$

1D Diffusion (Caution!)

Parabolic PDE

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1D Diffusion (Caution!)

Parabolic PDE

Characteristic lines are lines of constant 't'

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↓
All information at a given time should affect the solution

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Our Numerical Formulation:

$$u_i^{n+1} = u_i^n + \frac{\nu \Delta t}{\Delta x^2} (u_{i-1}^n - 2u_i^n + u_{i+1}^n)$$

1D Diffusion (Caution!)

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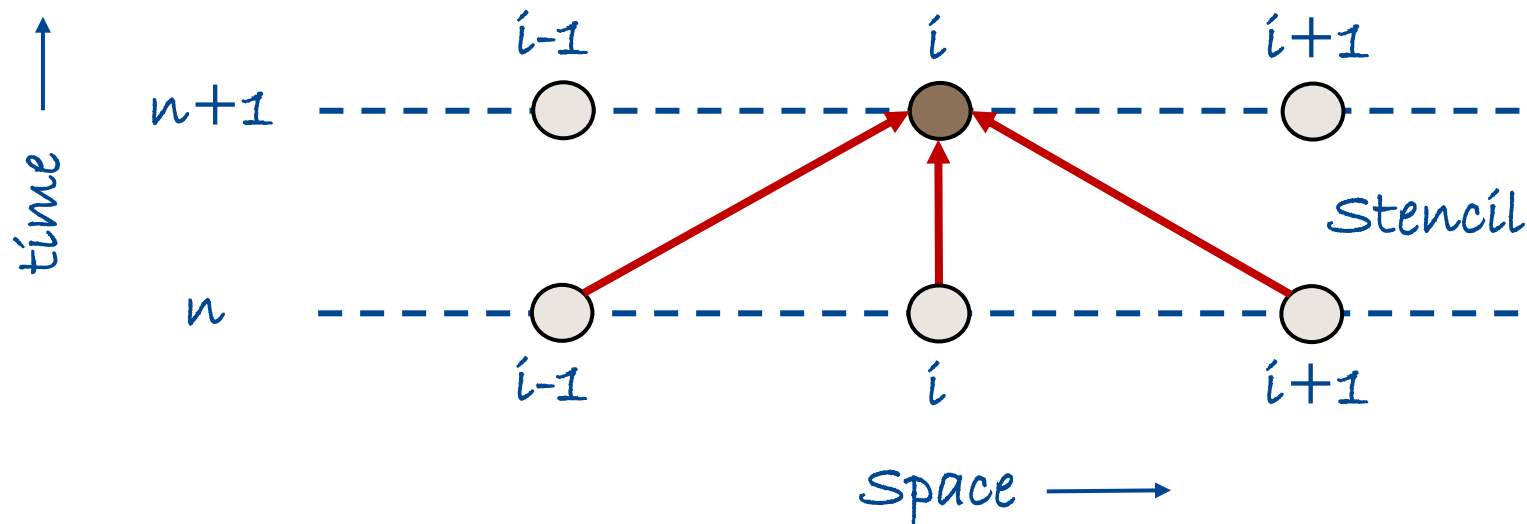
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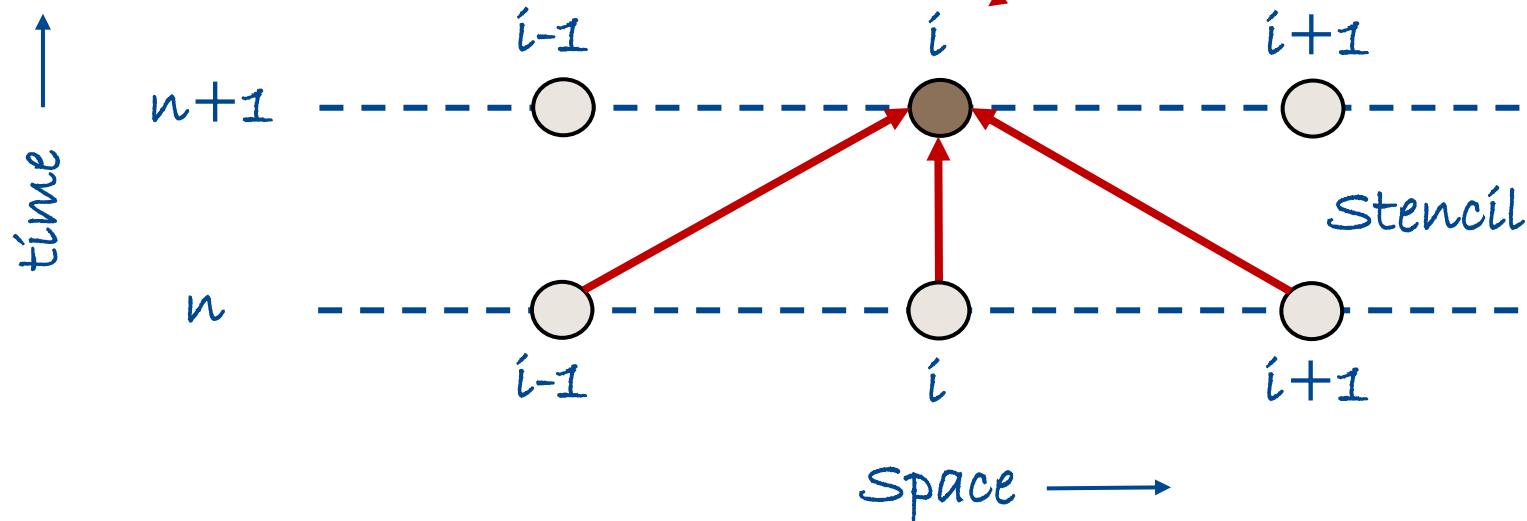
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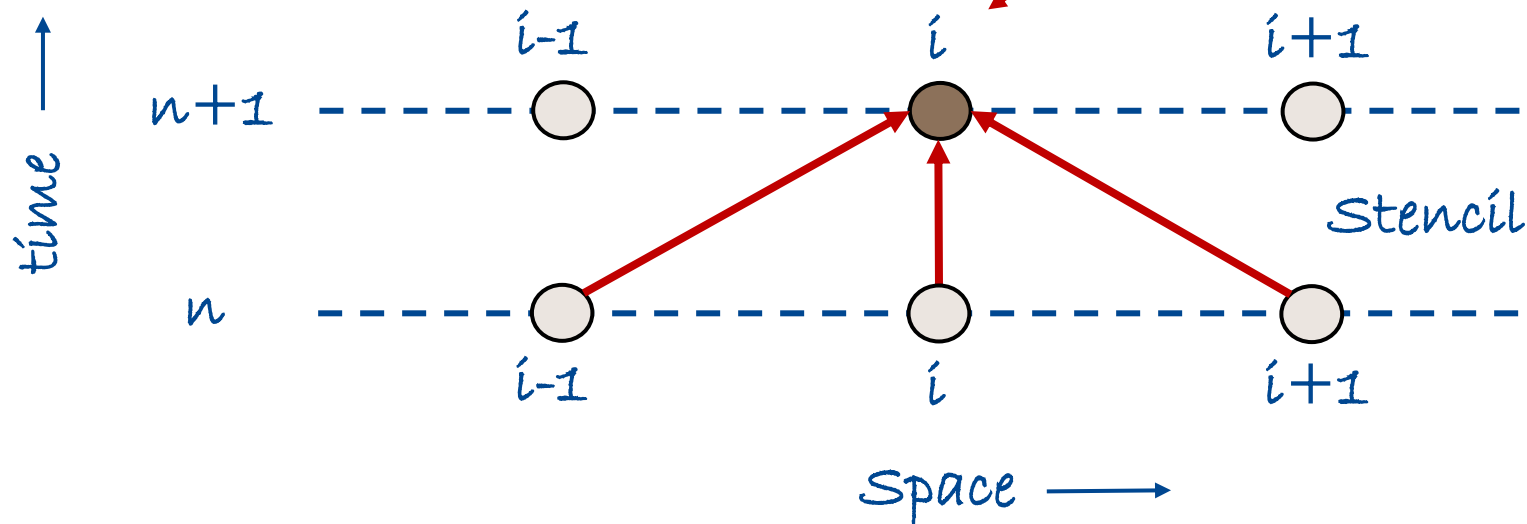
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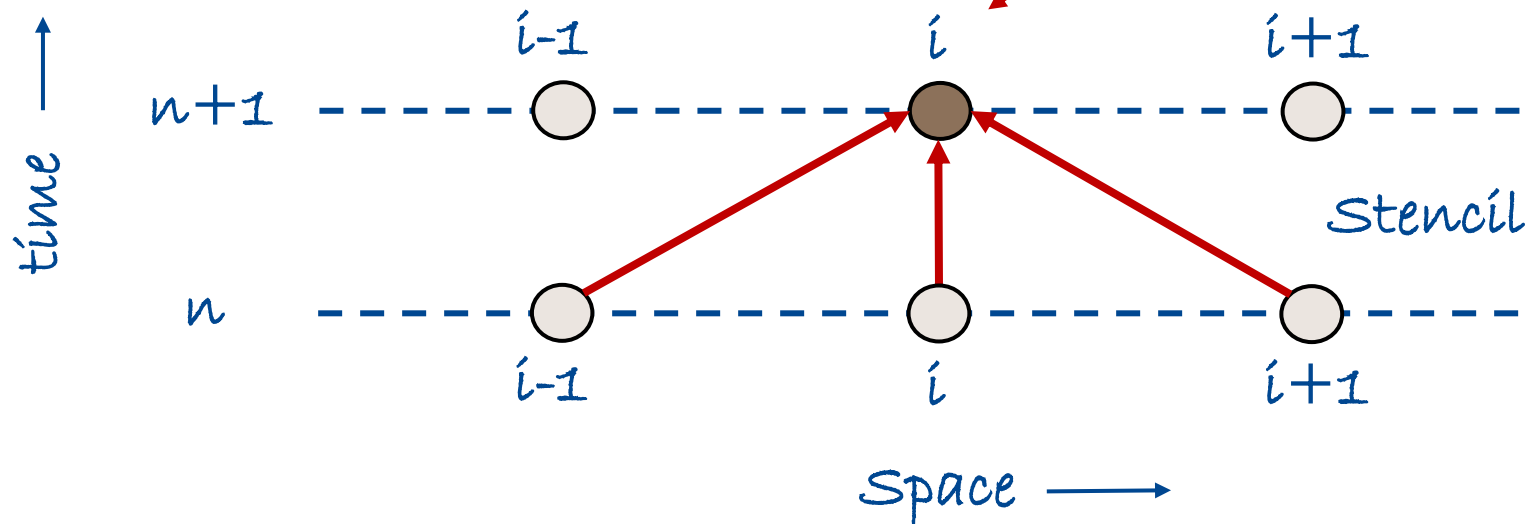
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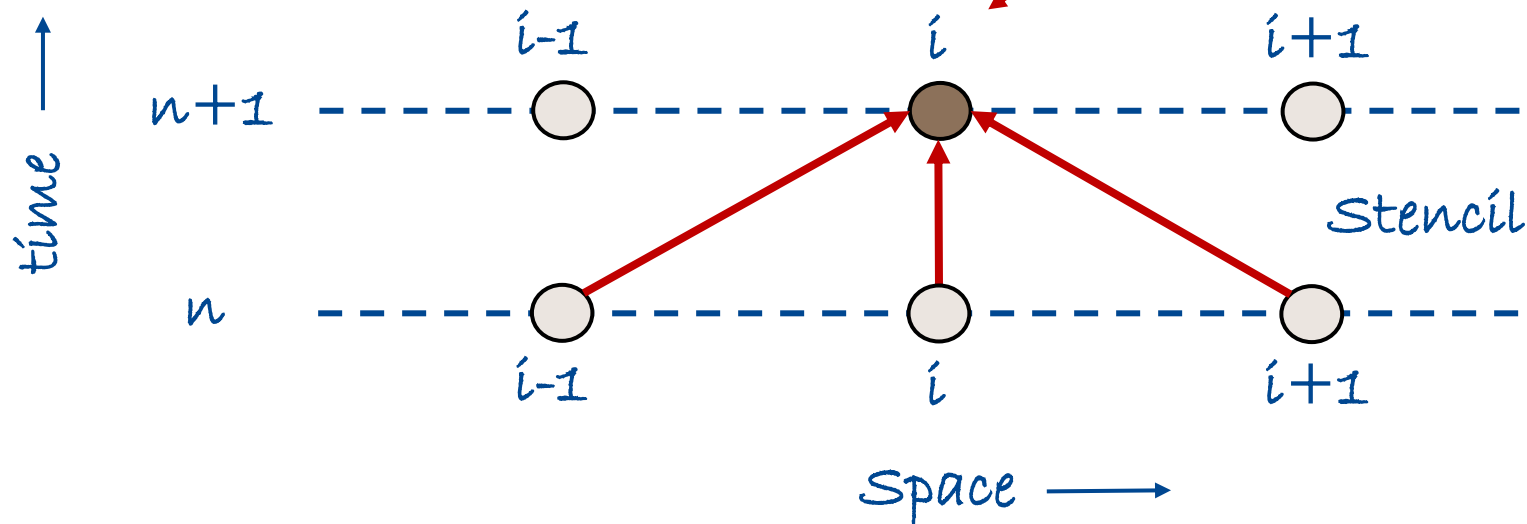
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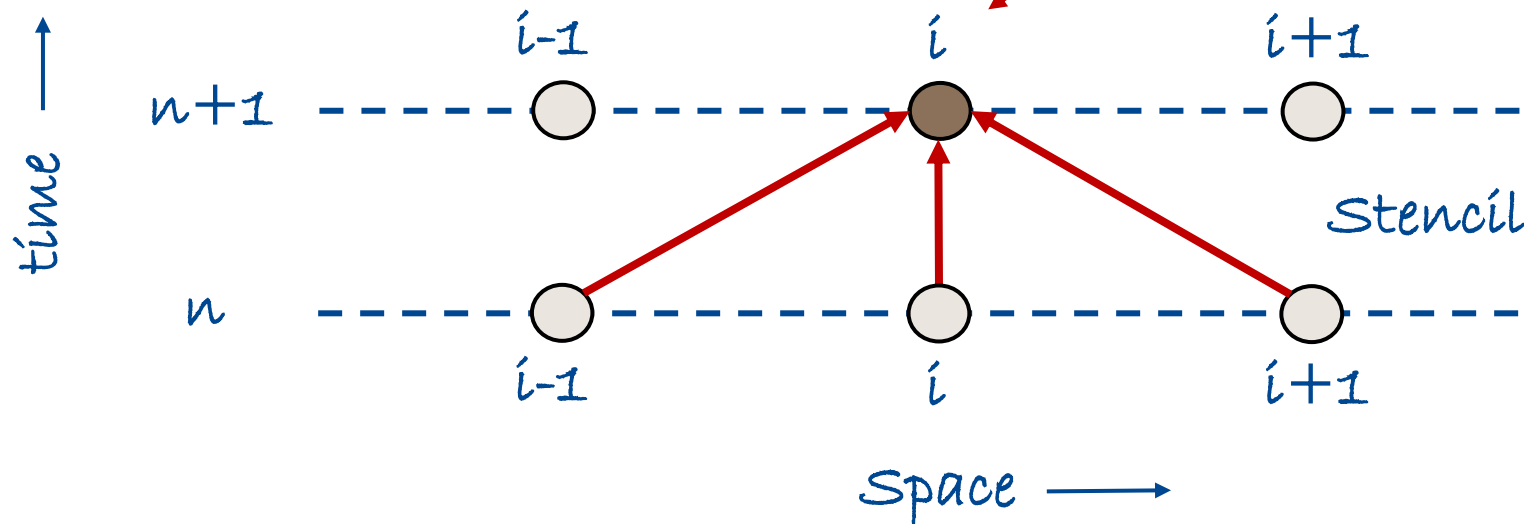
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How can we include BCs at current time?



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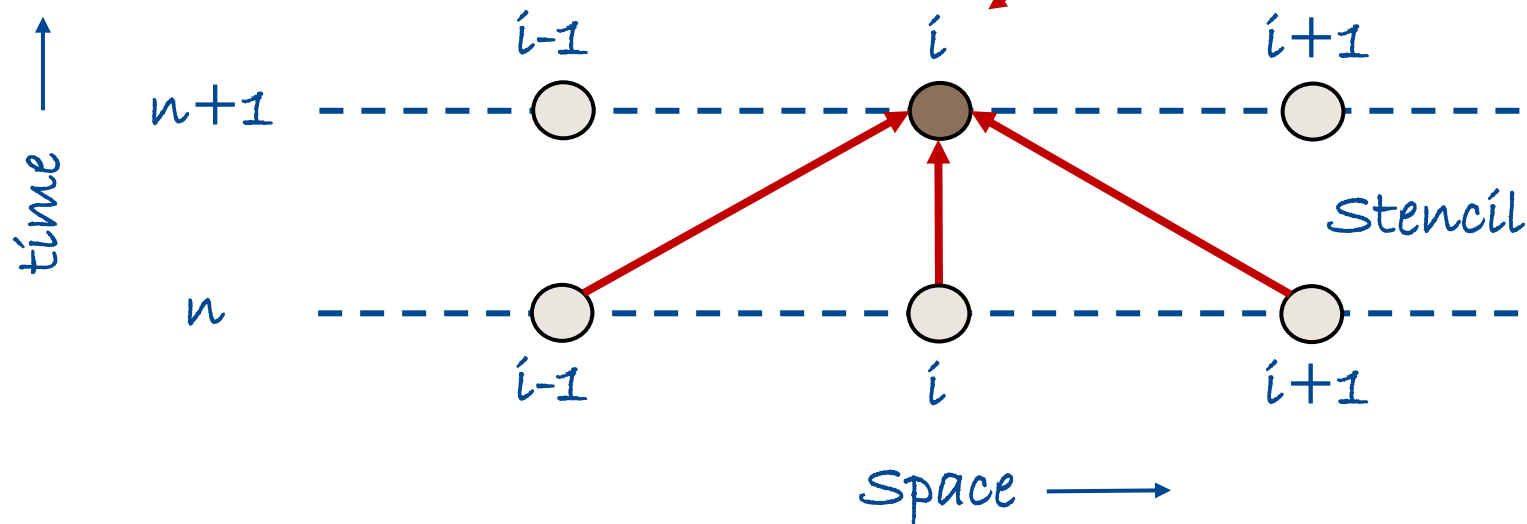
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1D Diffusion (Implicit Formulation)

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$$\frac{du}{dt} = \nu \frac{d^2 u}{dx^2} \quad \frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{\nu}{\Delta x^2} (u_{i-1}^n - 2u_i^n + u_{i+1}^n)$$

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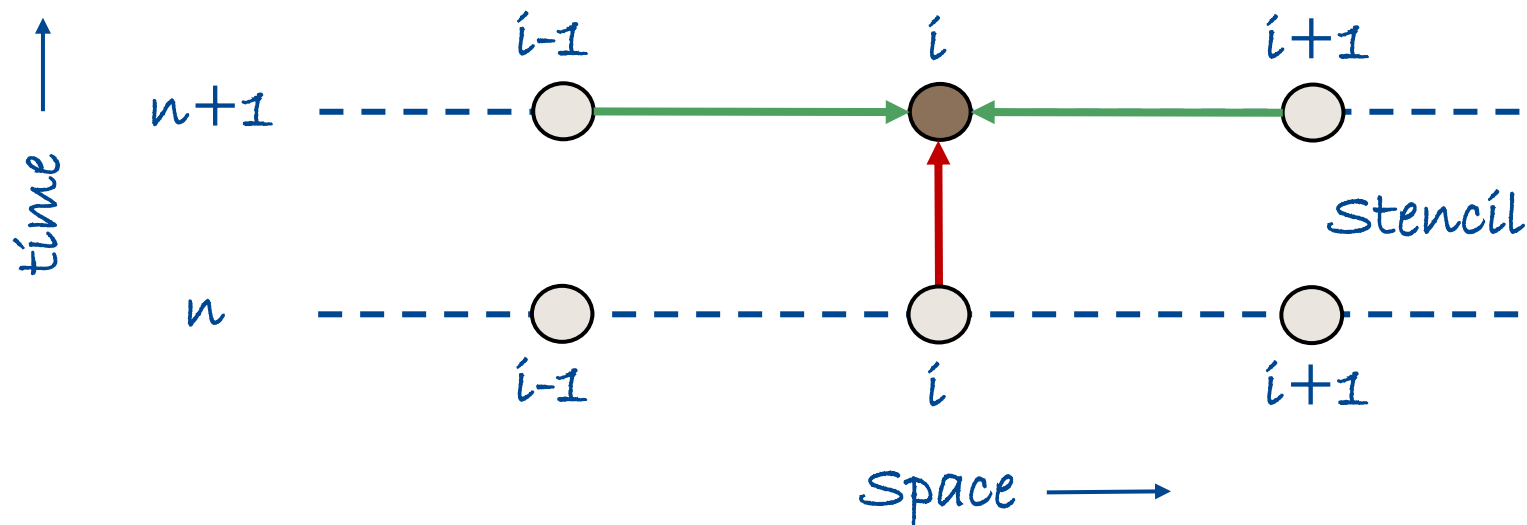
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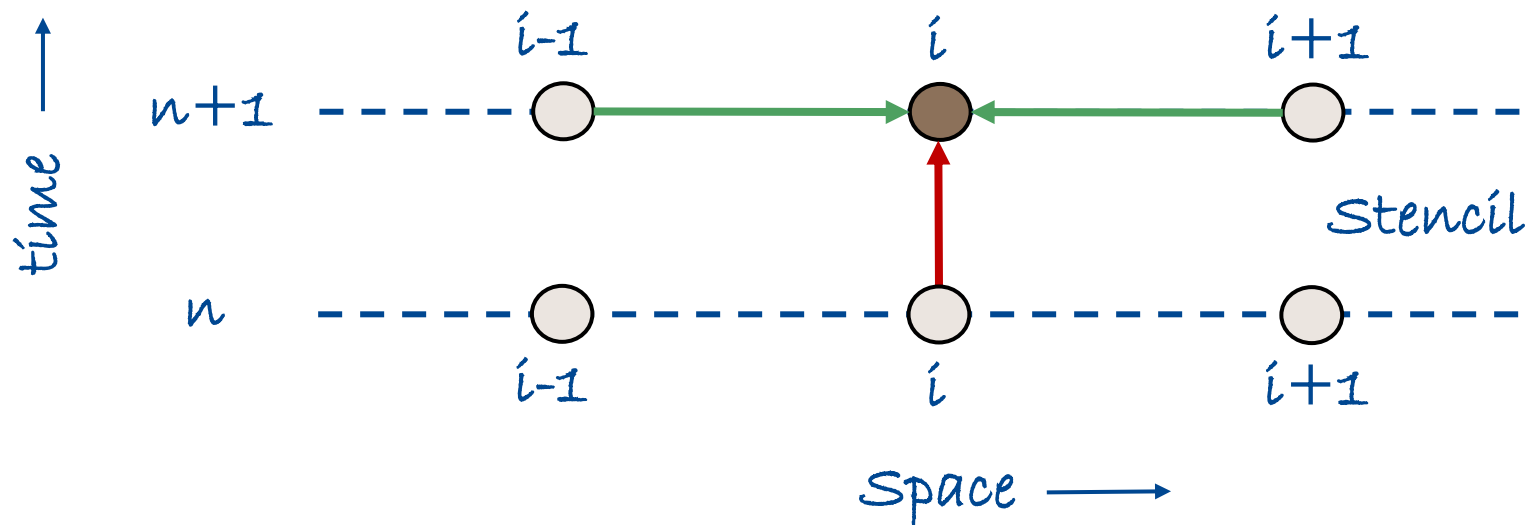
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1D Diffusion (Implicit Formulation)

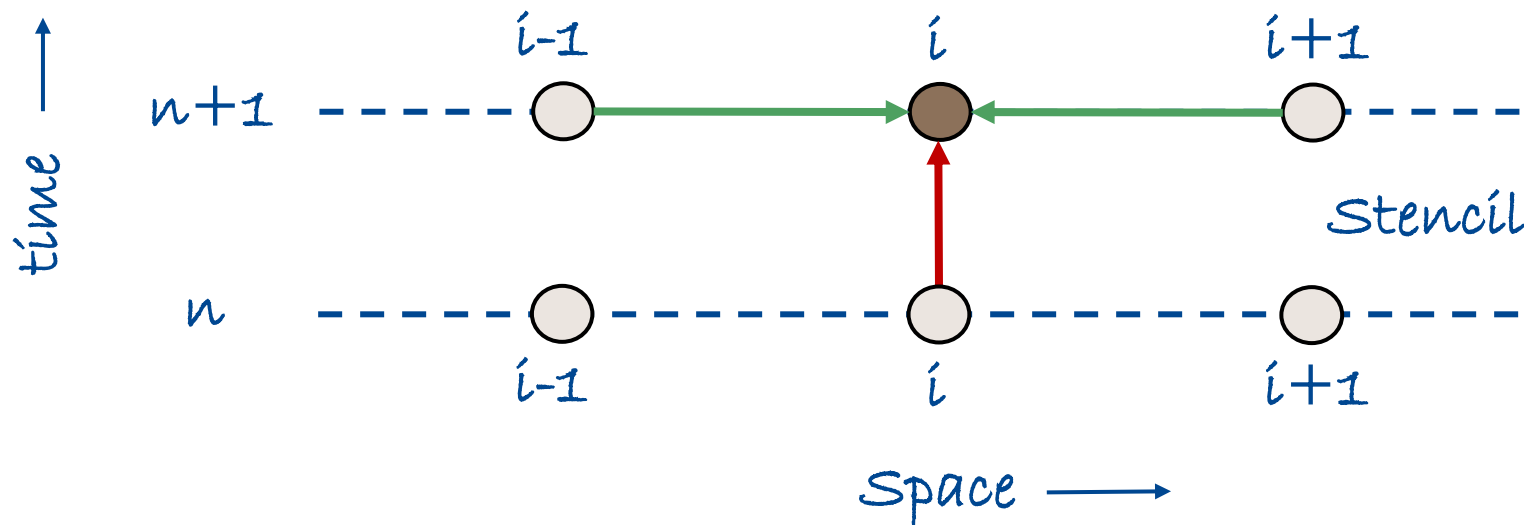
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Need Algorithms to solve such a sparse matrix system!



1D Diffusion (Implicit Formulation)

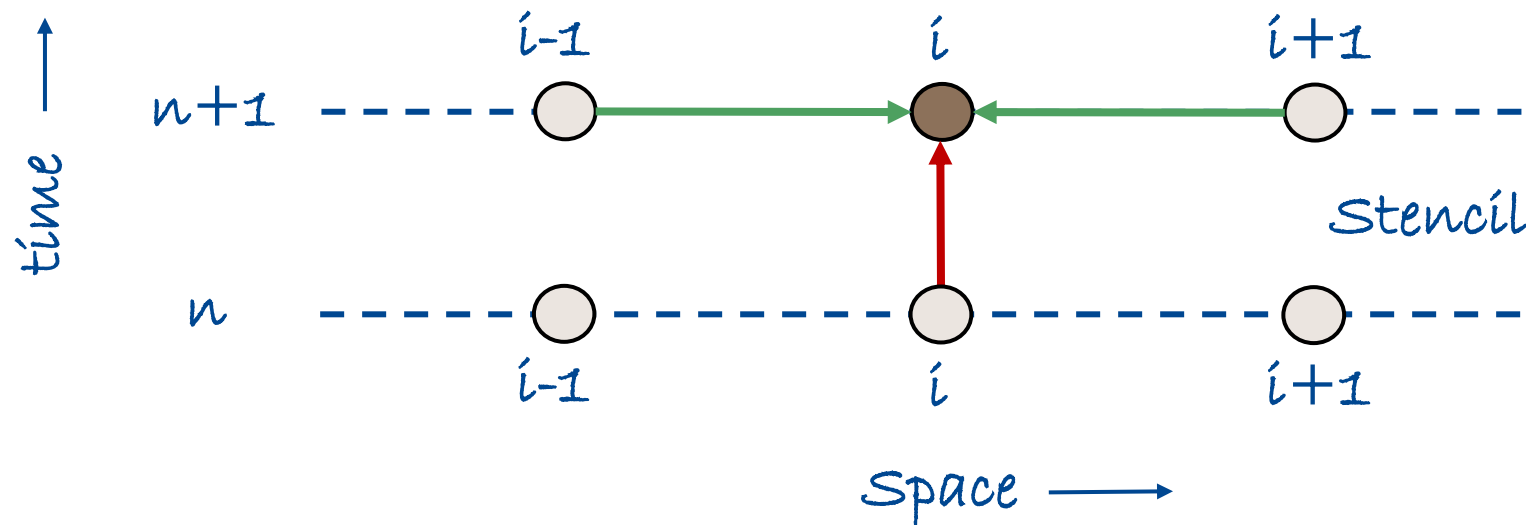
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Direct or Iterative
Methods

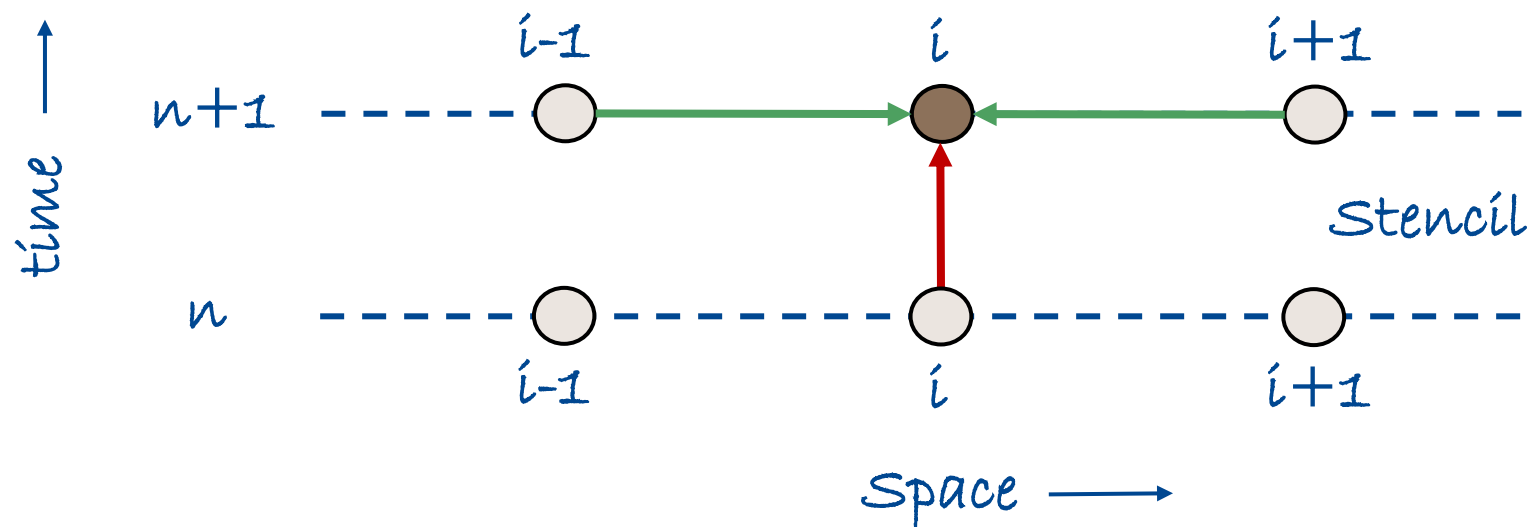
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Need Algorithms to solve such a sparse matrix system!

Direct or Iterative
Methods

Can be Expensive!

Crank-Nicholson Method

Well-known for Parabolic PDEs

$$\frac{1}{2} [\text{"Implicit Formulation"} + \text{"Explicit Formulation"}]$$

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Well-known for Parabolic PDEs

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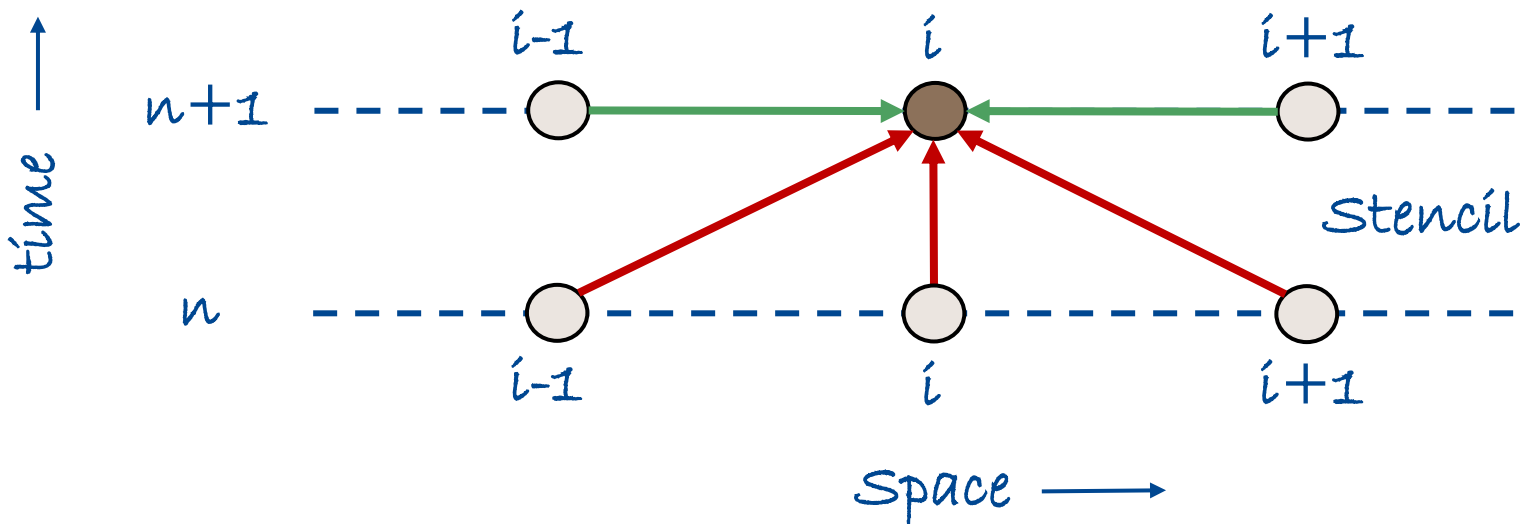
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{2} \left[\frac{\nu}{\Delta x^2} (u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}) + \frac{\nu}{\Delta x^2} (u_{i-1}^n - 2u_i^n + u_{i+1}^n) \right]$$

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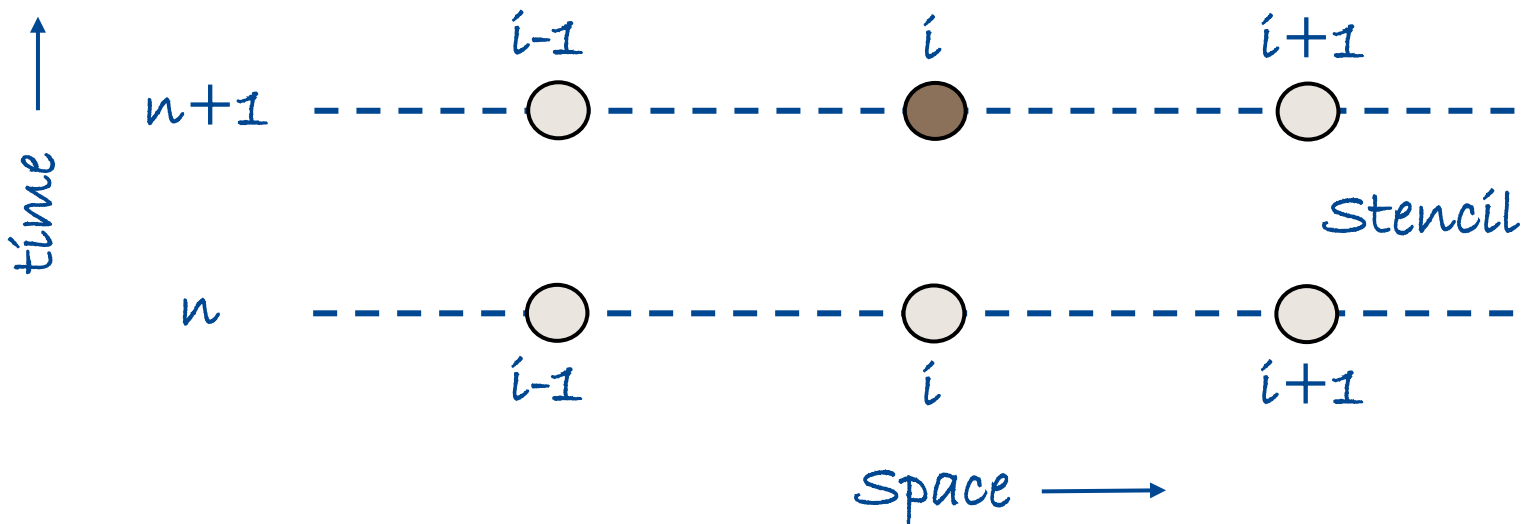


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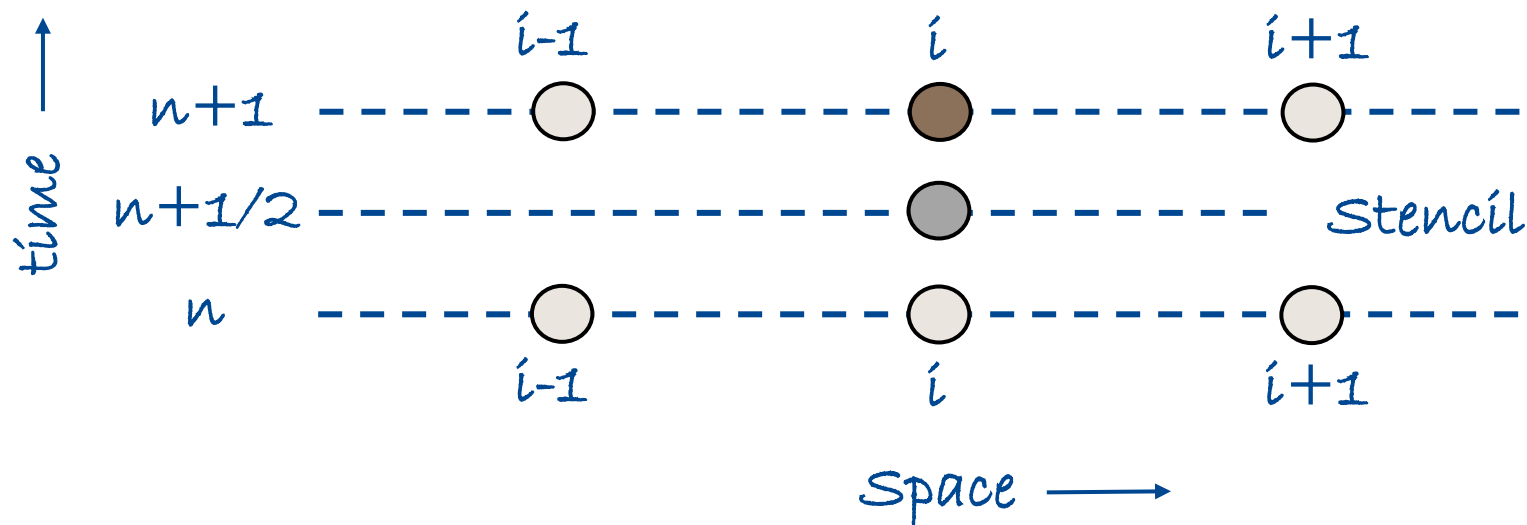


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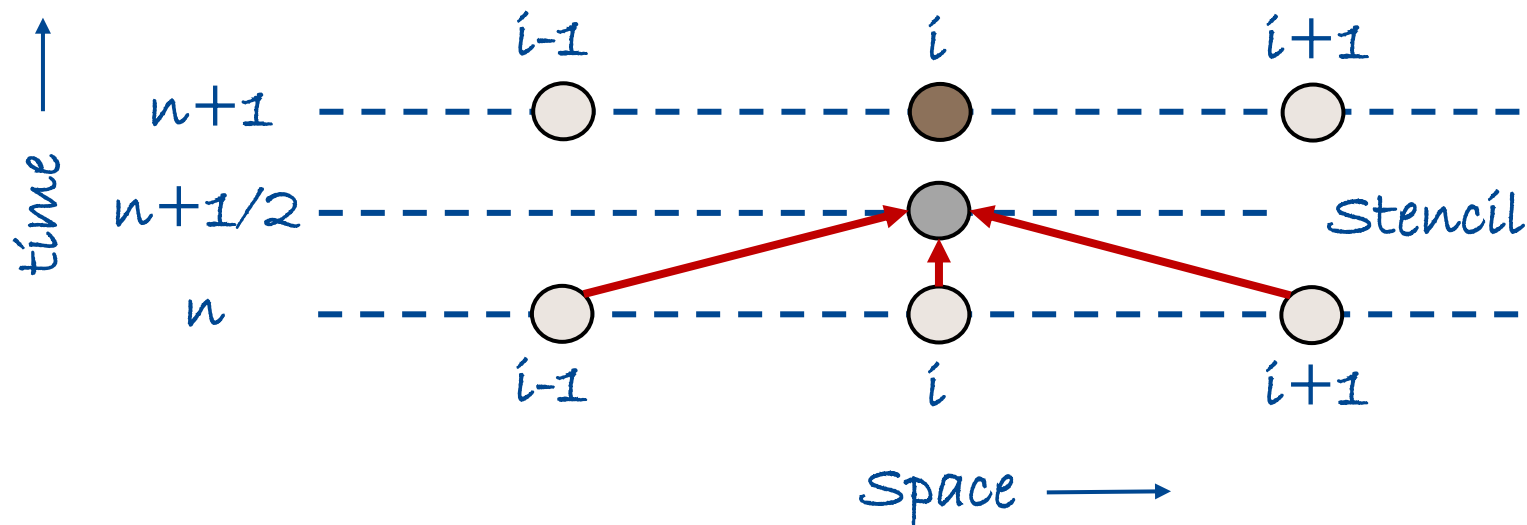


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$$\frac{1}{2} [\text{"Implicit Formulation"} + \text{"Explicit Formulation"}]$$

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Explicit:

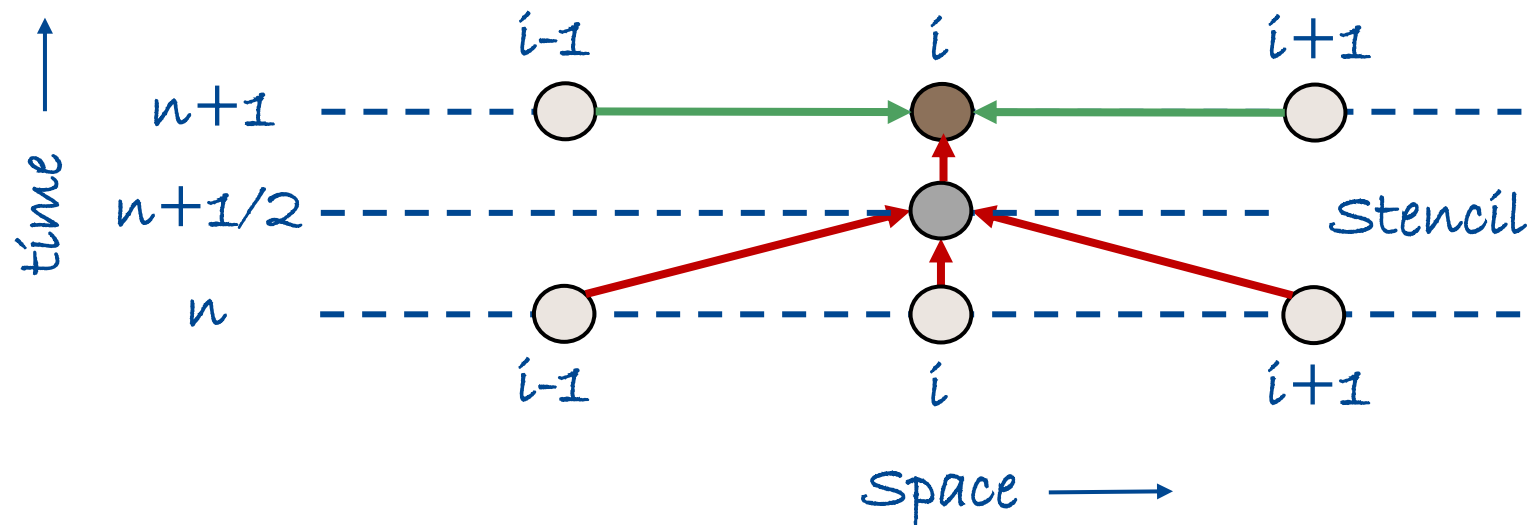
$$\frac{u_i^{n+1/2} - u_i^n}{\Delta t/2} = \frac{v}{\Delta x^2} (u_{i-1}^n - 2u_i^n + u_{i+1}^n)$$

Crank-Nicholson Method

Well-known for Parabolic PDEs

$$\frac{1}{2} [\text{"Implicit Formulation"} + \text{"Explicit Formulation"}]$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{2} \left[\frac{v}{\Delta x^2} (u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}) + \frac{v}{\Delta x^2} (u_{i-1}^n - 2u_i^n + u_{i+1}^n) \right]$$



Implicit:

$$\frac{u_i^{n+1} - u_i^{n+1/2}}{\Delta t/2} = \frac{v}{\Delta x^2} (u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1})$$

Explicit:

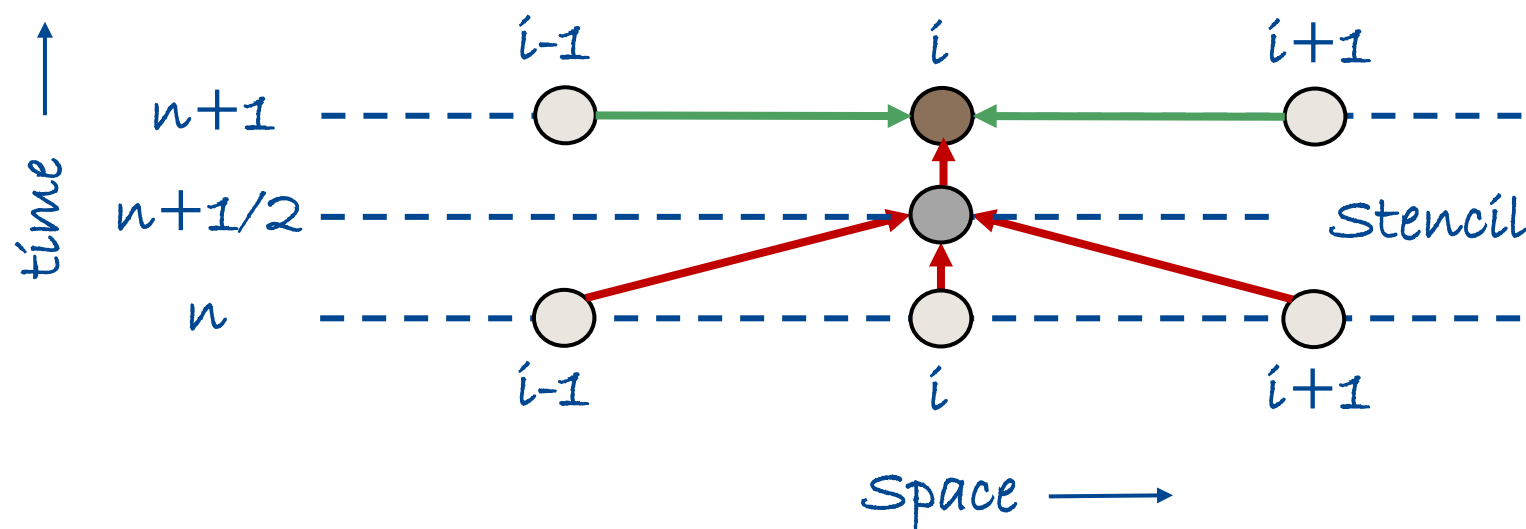
$$\frac{u_i^{n+1/2} - u_i^n}{\Delta t/2} = \frac{v}{\Delta x^2} (u_{i-1}^n - 2u_i^n + u_{i+1}^n)$$

Crank-Nicholson Method

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Implicit:

$$\frac{u_i^{n+1} - u_i^{n+1/2}}{\Delta t/2} = \frac{v}{\Delta x^2} (u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1})$$

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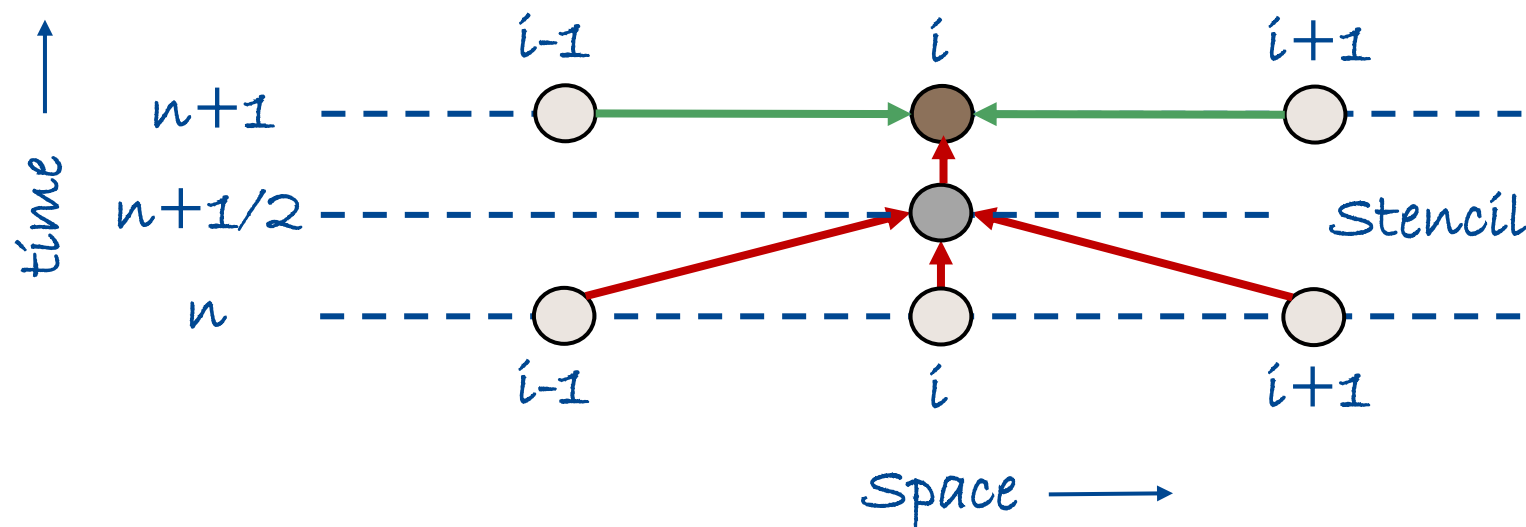
✓ 2nd order in time & space !

Crank-Nicholson Method

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✓ 2nd order in time & space!

⚠ Tridiagonal system to solve!

4th Code: 1D Burger's Equation

$$\frac{du}{dt} + u \frac{du}{dx} = \nu \frac{d^2u}{dx^2}$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + u_i^n \frac{u_i^n - u_{i-1}^n}{\Delta x} = \nu \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}$$

$$u_i^{n+1} = u_i^n - \frac{c\Delta t}{\Delta x} (u_i^n - u_{i-1}^n) + \frac{c\Delta t}{\Delta x^2} (u_{i-1}^n - 2u_i^n + u_{i-1}^n)$$

Initial Condition: $u(x, 0) = -\frac{2\nu}{\phi} \frac{\partial \phi}{\partial x} + 4$ $\phi = \exp\left(-\frac{x^2}{4\nu}\right) + \exp\left(-\frac{(x-2\pi)^2}{4\nu}\right)$ Boundary Condition: $u(0) = u(2\pi)$
Periodic BC!

Exact Solution: $u = -\frac{2\nu}{\phi} \frac{\partial \phi}{\partial x} + 4$ $\phi = \exp\left(-\frac{(x-4t)^2}{4\nu(t+1)}\right) + \exp\left(-\frac{(x-4t-2\pi)^2}{4\nu(t+1)}\right)$

Let's Code It!

4th Code: 1D Burger's Equation

```
import numpy as np
import sympy as sp
import pylab as pl
pl.ion()
```

4th Code: 1D Burger's Equation

```
import numpy as np
import sympy as sp
import pylab as pl
pl.ion()
```

```
x, nu, t = sp.symbols('x nu t')
phi = sp.exp(-(x-4*t)**2/(4*nu*(t+1))) + sp.exp(-(x-4*t-2*sp.pi)**2/(4*nu*(t+1)))
```

```
phiprime = phi.diff(x)
u = -2*nu*(phiprime/phi)+4
```

```
from sympy.utilities.lambdify import lambdify
ufunc = lambdify ((t, x, nu), u)
```

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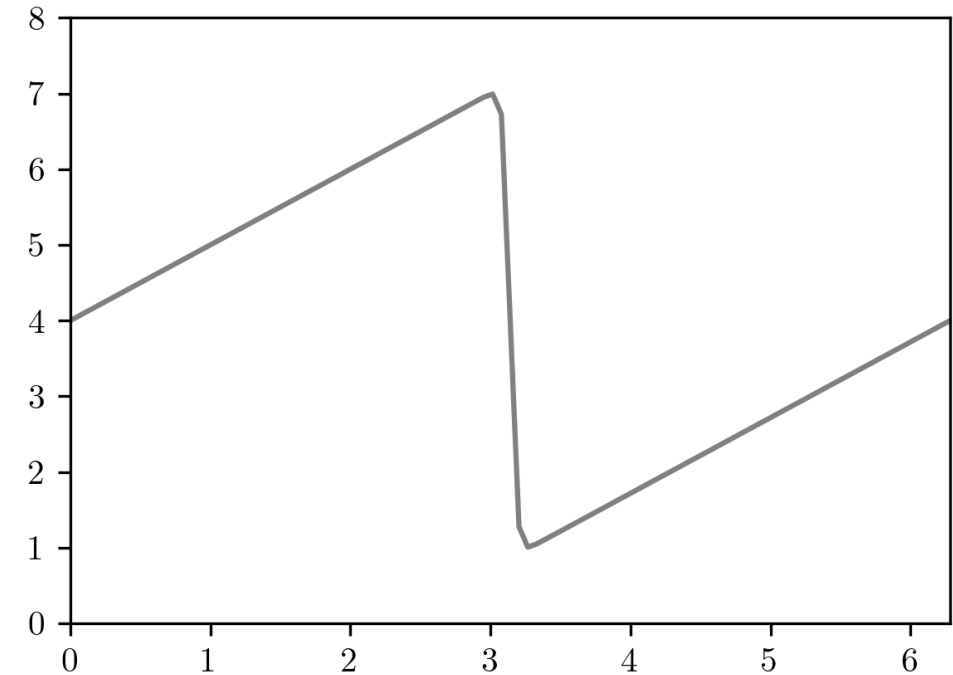
phiprime = phi.diff(x)
u = -2*nu*(phiprime/phi)+4

from sympy.utilities.lambdify import lambdify
ufunc = lambdify ((t, x, nu), u)

nx = 101
dx = 2*np.pi/(nx-1)
nt = 100
nu = 0.07
dt = dx*nu
T = nt*dt

grid = np.linspace(0, 2*np.pi, nx)
u = np.empty(nx)
t = 0
u = np.asarray([ufunc(t, x, nu) for x in grid])

pl.figure(figsize=(11,7), dpi=100)
pl.plot(grid,u, marker='o', lw=2)
pl.xlim([0,2*np.pi])
pl.ylim([0,10])
pl.xlabel('X')
pl.ylabel('Velocity')
pl.title('1D Burgers Equation - Initial condition')
```



4th Code: 1D Burger's Equation

```
import numpy as np
import sympy as sp
import pylab as pl
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```
x, nu, t = sp.symbols('x nu t')
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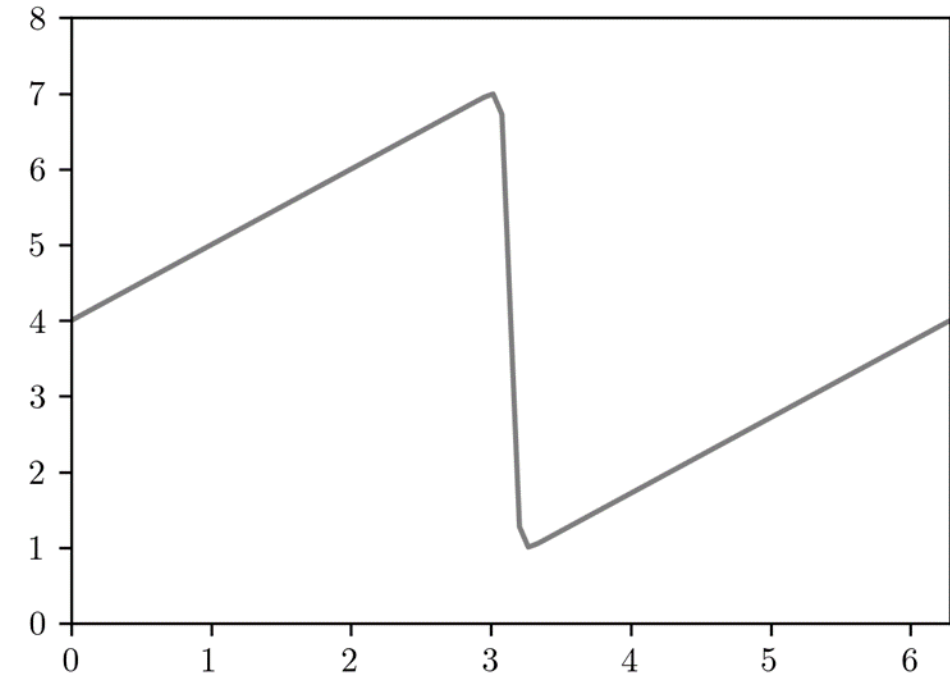
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pl.xlabel('X')
pl.ylabel('Velocity')
pl.title('1D Burgers Equation - Initial condition')
```

```
for n in range(nt):
    un = u.copy()
    for i in range(nx-1):
        u[i] = un[i] - un[i] * dt/dx * (un[i]-un[i-1]) + \
            nu * dt/(dx**2) * (un[i+1] - 2*un[i] + un[i-1])
    # infer the periodicity
    u[-1] = un[-1] - un[-1] * dt/dx * (un[-1]-un[-2]) + \
        nu * dt/(dx**2) * (un[0] - 2*un[-1] + un[-2])
```

```
u_analytical = np.asarray([ufunc(T, xi, nu) for xi in grid])
```

```
pl.figure(figsize=(11,7), dpi=100)
pl.plot(grid, u, marker='o', lw=2, label='Computational')
pl.plot(grid, u_analytical, label='Analytical')
pl.xlim([0, 2*np.pi])
pl.ylim([0,10])
pl.legend()
pl.xlabel('X')
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pl.title('1D Burgers Equation - Solutions')
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4th Code: 1D Burger's Equation

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import numpy as np
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```
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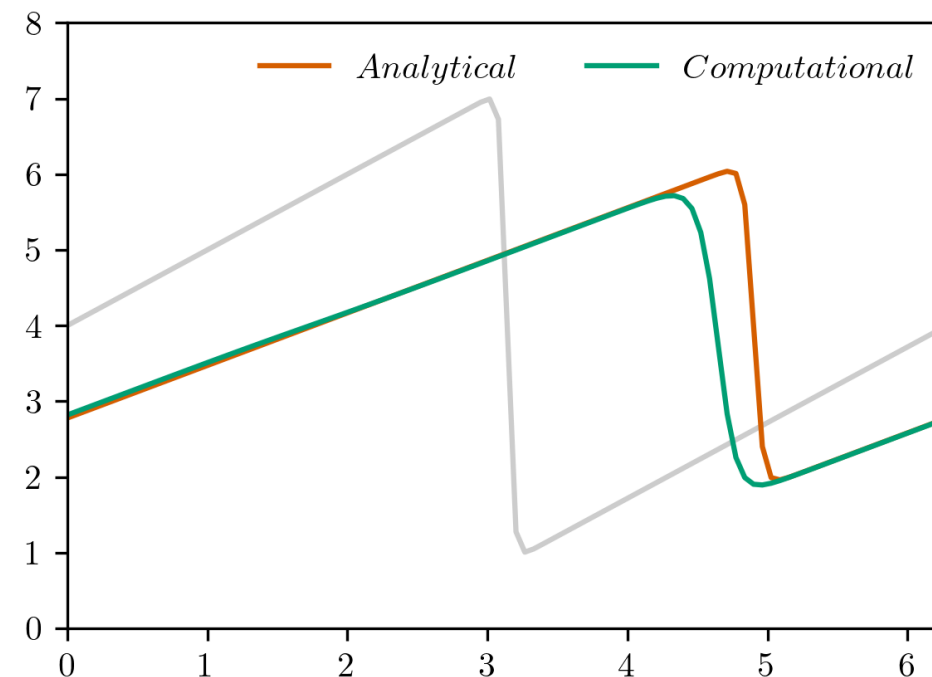
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5th Code: 2D Laplace Equation

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} = 0$$

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$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} = 0$$

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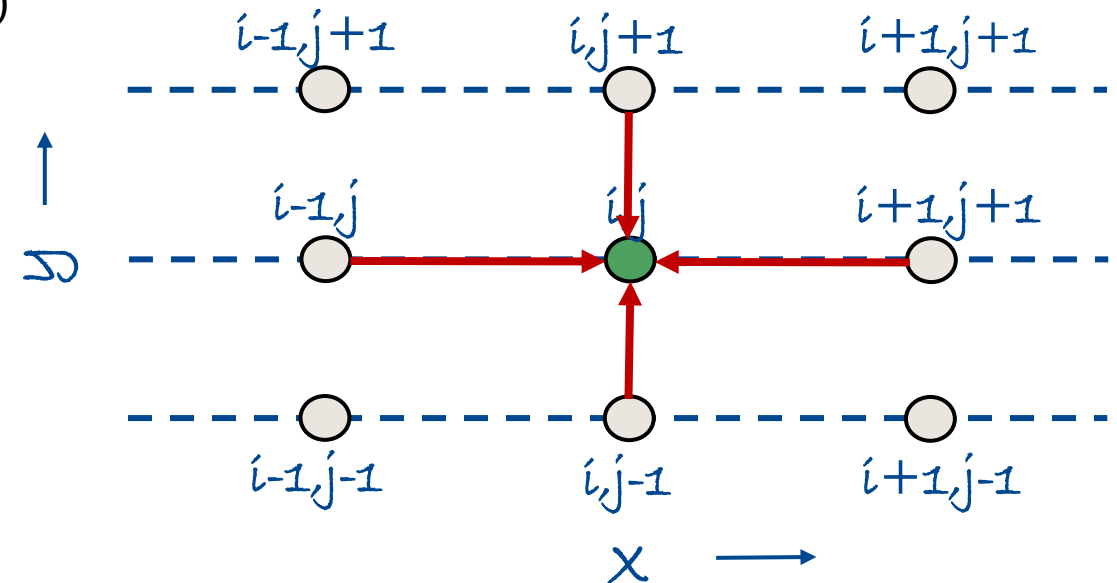
5th Code: 2D Laplace Equation

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5 points stencil



5th Code: 2D Laplace Equation

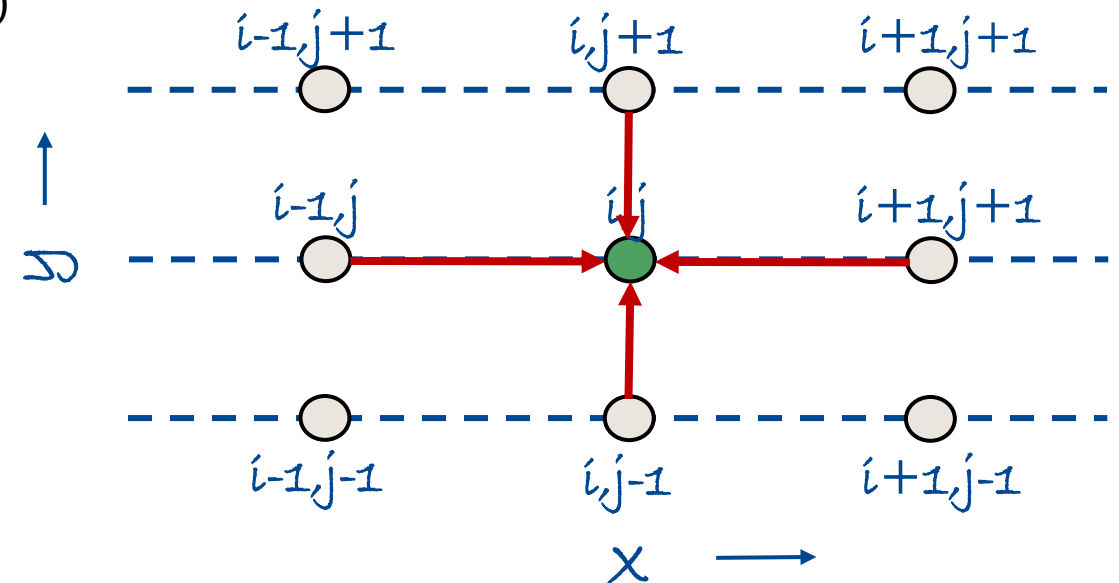
No time dependence !

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5th Code: 2D Laplace Equation

Calculates an
equilibrium state
given the specified BCs

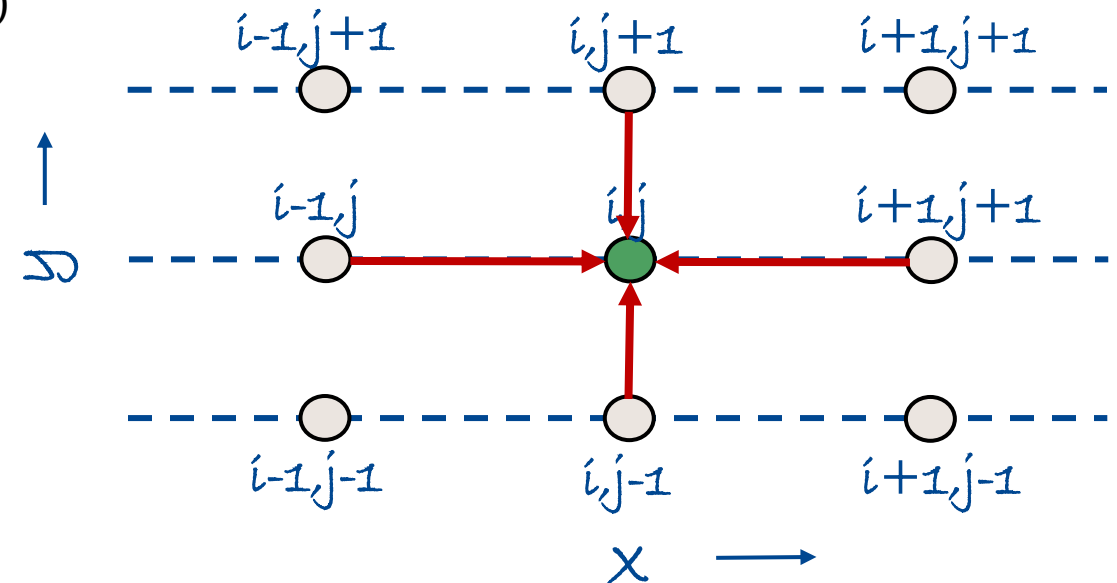
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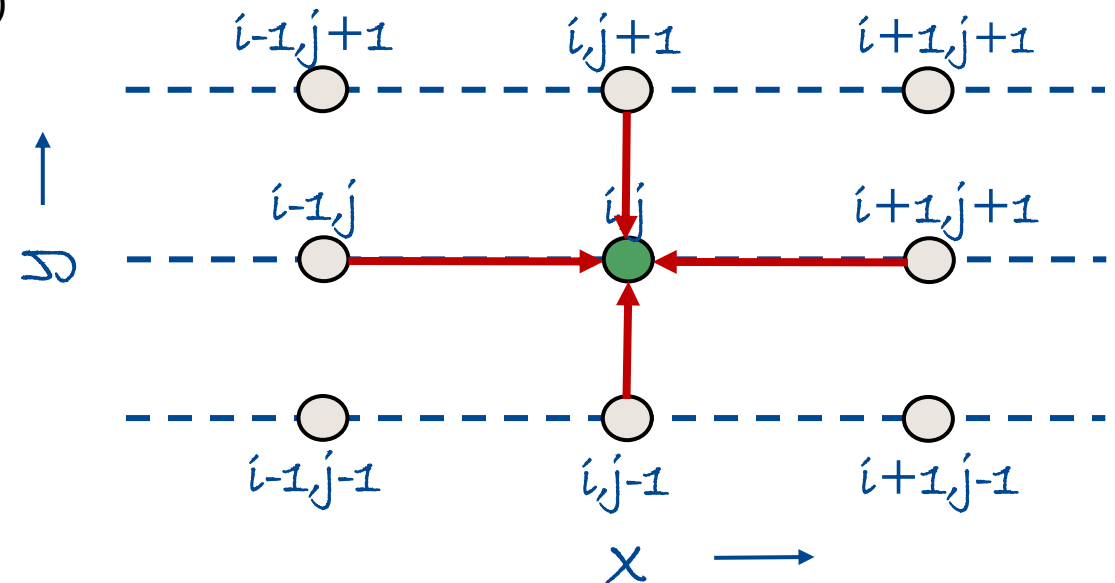
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5 points stencil

Need to solve iteratively

Will reach equilibrium as
iterations $\rightarrow \infty$

Need to specify a threshold!



5th Code: 2D Laplace Equation

Calculates an
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No time dependence !

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} = 0 \quad \text{BCs:} \quad \begin{aligned} p &= 0 \text{ at } x = 0 \\ p &= y \text{ at } x = 2 \end{aligned} \quad \frac{\partial p}{\partial y} = 0 \text{ at } y = 0, 1$$

$$\frac{p_{i+1,j}^n - 2p_{i,j}^n + p_{i-1,j}^n}{\Delta x^2} + \frac{p_{i,j+1}^n - 2p_{i,j}^n + p_{i,j-1}^n}{\Delta y^2} = 0$$

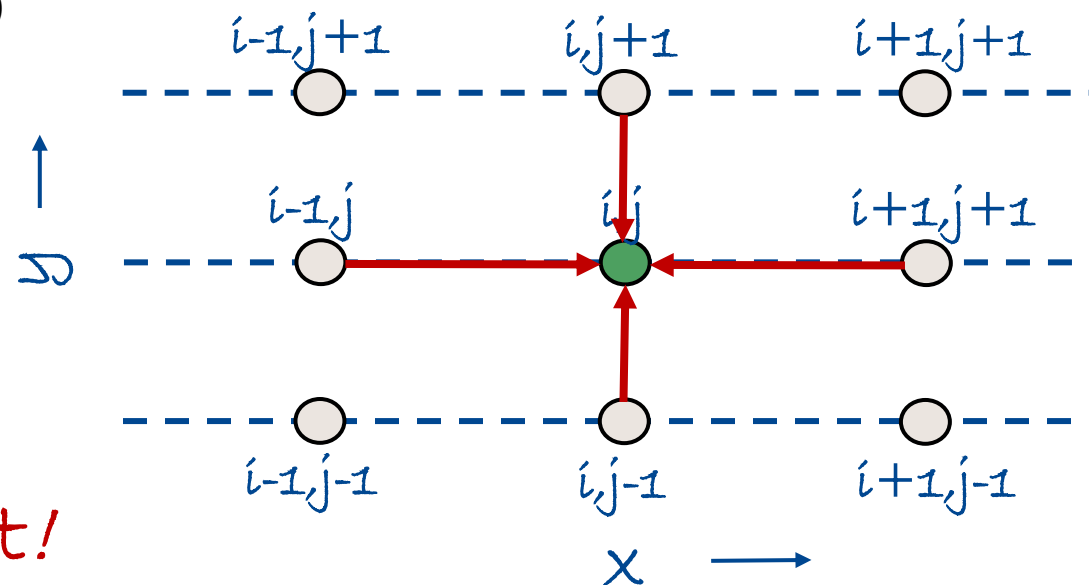
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Let's Code it!

5th Code: 2D Laplace Equation

Calculates an
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No time dependence !

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} = 0$$

BCs:

$$p = 0 \text{ at } x = 0$$

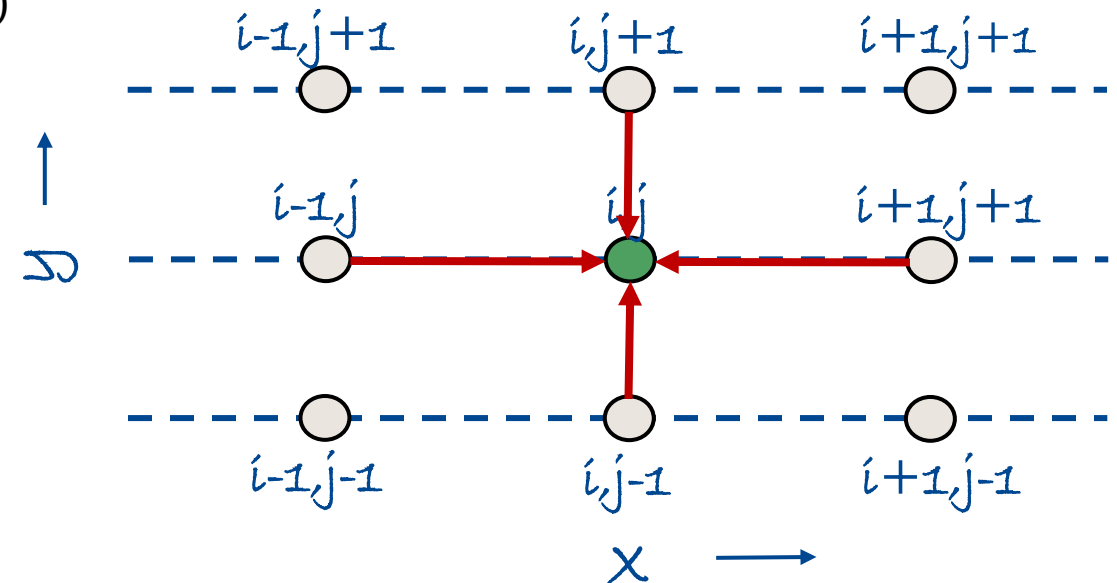
$$p = y \text{ at } x = 2$$

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5th Code: 2D Laplace Equation

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



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def plot2D(x,y,p):
    fig = pyplot.figure( figsize=(11,7), dpi=100 )
    ax = fig.gca(projection='3d')
    X, Y = np.meshgrid(x,y)
    surf = ax.plot_surface( X, Y, p[:,], rstride=1, cstride=1, cmap=cm.viridis,
                           linewidth=0, antialiased=False )
    ax.set_xlabel("$x$"); ax.set_xlim(0,2)
    ax.set_ylabel("$y$"); ax.set_ylim(0,1)
    ax.view_init(30,225)
```

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    ax.view_init(30,225)

def laplace2D(p,y,dx,dy,target_norm):
    norm=1
    pn = np.empty_like(p)
    while norm > target_norm:
        pn = p.copy()
        p[1:-1,1:-1] = (
            (dy**2 * (pn[1:-1,2:] - pn[1:-1,-2])) +
            (dx**2 * (pn[2:,1:-1] - pn[-2,1:-1]))
        ) / (2 * (dx**2 + dy**2))
        p[:,0] = 0 # p=0 at x=0
        p[:,-1] = y # p=y at x=2
        p[0,:] = p[1,:] # dp/dy=0 at y=0
        p[-1,:] = p[-2,:] # dp/dy=0 at y=1
        norm = (np.sum(np.abs(p)) - np.sum(np.abs(pn)))/(np.sum(np.abs(pn)))
    return p
```

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        p[-1,:] = p[-2,:] # dp/dy=0 at y=1
        norm = (np.sum(np.abs(p)) - np.sum(np.abs(pn)))/(np.sum(np.abs(pn)))
    return p

nx = 31; ny = 31; dx = 2/(nx-1); dy = 1/(ny-1)
x = np.linspace(0, 2, nx); y = np.linspace(0, 1, ny)
```

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from matplotlib import pyplot, cm
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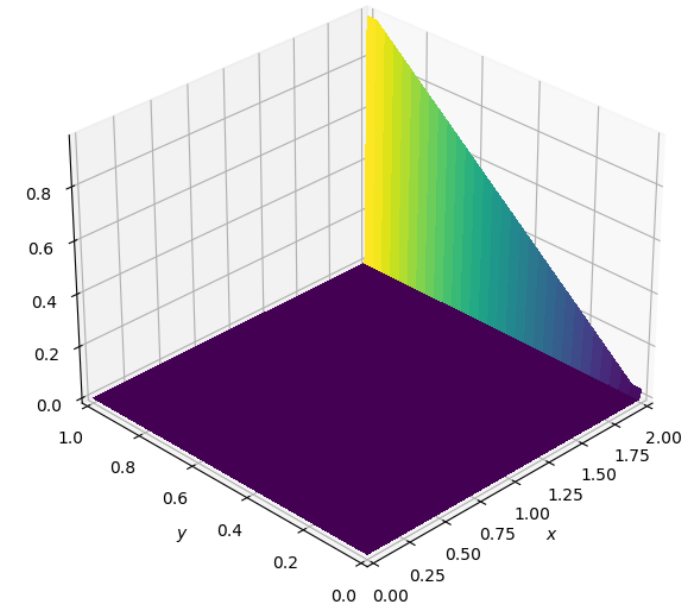
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        p[:,0] = 0 # p=0 at x=0
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        p[0,:] = p[1,:] # dp/dy=0 at y=0
        p[-1,:] = p[-2,:] # dp/dy=0 at y=1
        norm = (np.sum(np.abs(p)) - np.sum(np.abs(pn)))/(np.sum(np.abs(pn)))
    return p

nx = 31; ny = 31; dx = 2/(nx-1); dy = 1/(ny-1)
x = np.linspace(0, 2, nx); y = np.linspace(0, 1, ny)
```

```
p = np.zeros((ny,nx))
p[:,0] = 0 # p=0 at x=0
p[:,-1] = y # p=y at x=2
p[0,:] = p[1,:] # dp/dy=0 at y=0
p[-1,:] = p[-2,:] # dp/dy=0 at y=1

plot2D(x,y,p)
```



5th Code: 2D Laplace Equation

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

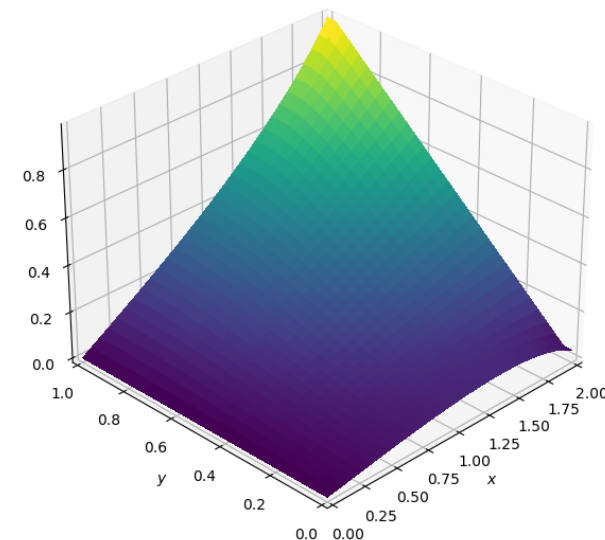
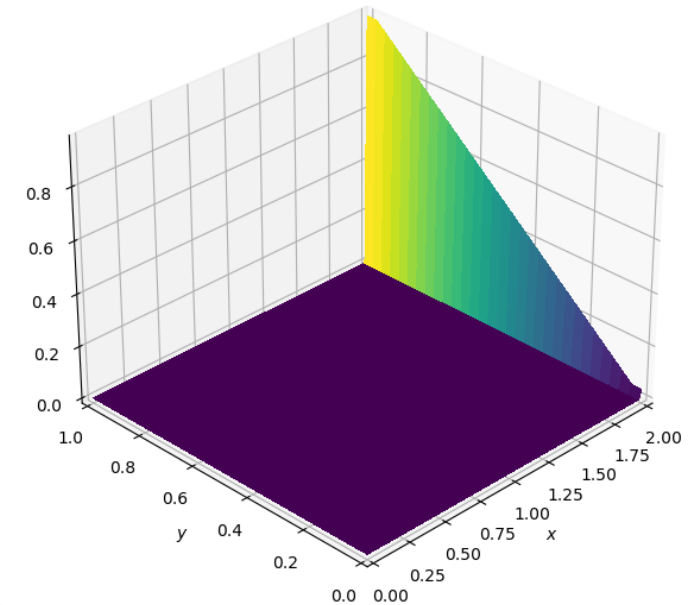
```
def plot2D(x,y,p):
    fig = pyplot.figure( figsize=(11,7), dpi=100 )
    ax = fig.gca(projection='3d')
    X, Y = np.meshgrid(x,y)
    surf = ax.plot_surface( X, Y, p[:,], rstride=1, cstride=1, cmap=cm.viridis,
                           linewidth=0, antialiased=False )
    ax.set_xlabel("$x$"); ax.set_xlim(0,2)
    ax.set_ylabel("$y$"); ax.set_ylim(0,1)
    ax.view_init(30,225)
```

```
def laplace2D(p,y,dx,dy,target_norm):
    norm=1
    pn = np.empty_like(p)
    while norm > target_norm:
        pn = p.copy()
        pn[1:-1,1:-1] = (
            (dy**2 * (pn[1:-1,2:] + pn[1:-1,-2])) +
            (dx**2 * (pn[2:,1:-1] + pn[-2,1:-1]))
        ) / (2 * (dx**2 + dy**2))
        pn[:,0] = 0 # p=0 at x=0
        pn[:, -1] = y # p=y at x=2
        pn[0,:] = pn[1,:] # dp/dy=0 at y=0
        pn[-1,:] = pn[-2,:] # dp/dy=0 at y=1
        norm = (np.sum(np.abs(p)) - np.sum(np.abs(pn)))/(np.sum(np.abs(pn)))
    return p
```

```
nx = 31; ny = 31; dx = 2/(nx-1); dy = 1/(ny-1)
x = np.linspace(0, 2, nx); y = np.linspace(0, 1, ny)
```

```
p = np.zeros((ny,nx))
p[:,0] = 0 # p=0 at x=0
p[:, -1] = y # p=y at x=2
p[0,:] = p[1,:] # dp/dy=0 at y=0
p[-1,:] = p[-2,:] # dp/dy=0 at y=1
```

```
plot2D(x,y,p)
p = laplace2D(p,y,dx,dy,1e-4)
plot2D(x,y,p)
```



Navier-Stokes equations for incompressible flows

Continuity equation:

$$\nabla \cdot \vec{v} = 0$$

Momentum equation:

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \vec{v}$$

Navier-Stokes equations for incompressible flows

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No equation for pressure !

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No equation for pressure !

There is no obvious way of coupling these equations !

Navier-Stokes equations for incompressible flows

Continuity equation:

$$\nabla \cdot \vec{v} = 0 \quad \longleftarrow$$

Provides a kinematic constraint that requires pressure field to evolve such that the velocity field remains solenoidal !

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Such a relation can be obtained by taking the divergence of the momentum equation.

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Such a relation can be obtained by taking the divergence of the momentum equation.

$$\nabla \cdot \left(\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} \right) = \nabla \cdot (-\nabla p + \nu \nabla^2 \vec{v})$$

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$$\nabla \cdot \left(\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} \right) = \nabla \cdot (-\nabla p + \nu \nabla^2 \vec{v})$$

$$\cancel{\frac{\partial \nabla \cdot \vec{v}}{\partial t}} + \nabla \cdot (\vec{v} \cdot \nabla) \vec{v} = -\nabla^2 p + \nu \nabla^2 \cancel{\nabla \cdot \vec{v}}$$

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$$\cancel{\frac{\partial \nabla \cdot \vec{v}}{\partial t}} + \nabla \cdot (\vec{v} \cdot \nabla) \vec{v} = -\nabla^2 p + \nu \cancel{\nabla^2 \nabla \cdot \vec{v}}$$

$$\nabla^2 p = -\nabla \cdot (\vec{v} \cdot \nabla) \vec{v}$$

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Pressure Poisson Equation

$$\nabla^2 p = -\nabla \cdot (\vec{v} \cdot \nabla) \vec{v}$$

Remedy: "Construct" a pressure field that guarantees continuity constraint!

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Continuity equation:

$$\nabla \cdot \vec{v} = 0 \quad \longleftarrow$$

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Momentum equation:

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Such a relation can be obtained by taking the divergence of the momentum equation.

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$$\cancel{\frac{\partial \nabla \cdot \vec{v}}{\partial t}} + \nabla \cdot (\vec{v} \cdot \nabla) \vec{v} = -\nabla^2 p + \nu \nabla^2 \cancel{\nabla \cdot \vec{v}}$$

Pressure Poisson Equation

$$\nabla^2 p = -\nabla \cdot (\vec{v} \cdot \nabla) \vec{v}$$

Let's look at the 6th code to learn how to solve a Poisson's equation.

Remedy: "Construct" a pressure field that guarantees continuity constraint!

6th Code: 2D Poisson's Equation

Obtained by adding a source term on the right-hand side of the Laplace's equation

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} = b$$

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Poisson's equation act to "relax" the initial sources in the field

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Poisson's equation act to "relax" the initial sources in the field

Discretized form:

$$\frac{p_{i+1,j}^n - 2p_{i,j}^n + p_{i-1,j}^n}{\Delta x^2} + \frac{p_{i,j+1}^n - 2p_{i,j}^n + p_{i,j-1}^n}{\Delta y^2} = b_{i,j}^n$$

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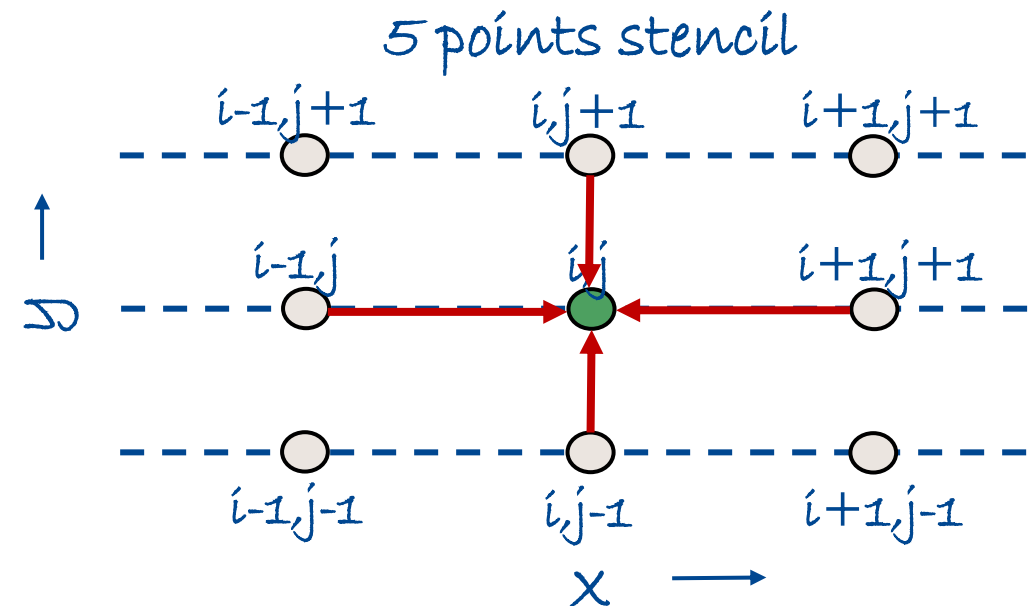
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$$p_{i,j}^n = \frac{\Delta y^2(p_{i+1,j}^n + p_{i-1,j}^n) + \Delta x^2(p_{i,j+1}^n + p_{i,j-1}^n) - b_{i,j}^n \Delta x^2 \Delta y^2}{2(\Delta x^2 + \Delta y^2)}$$



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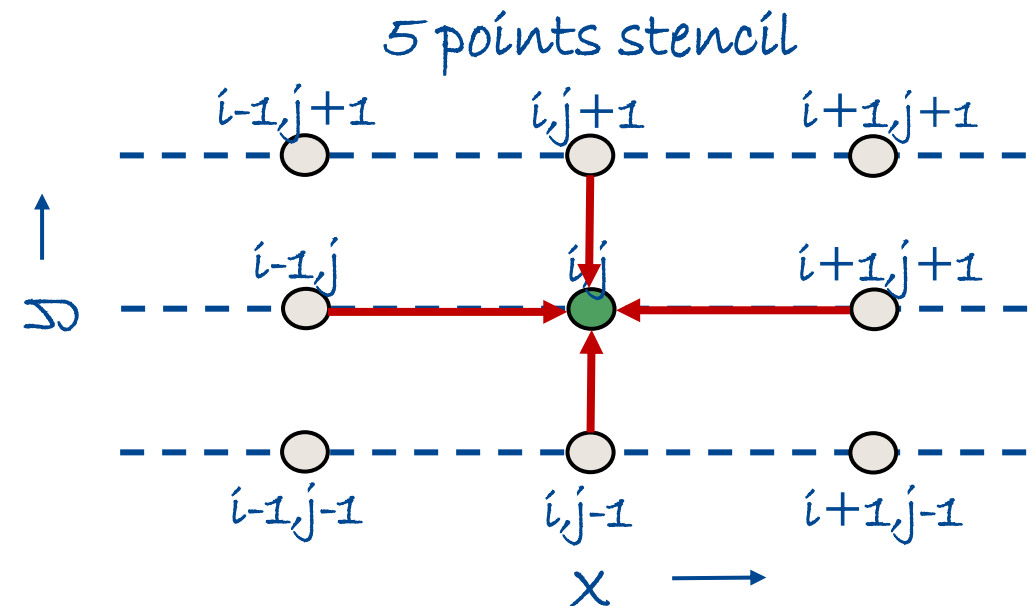
Source term:

$$b_{i,j} = -100 \text{ at } i = \frac{nx}{4}, j = \frac{ny}{4}$$

2 Spikes

$$b_{i,j} = 100 \text{ at } i = \frac{3nx}{4}, j = \frac{ny}{4}$$

$$b_{i,j} = 0 \text{ elsewhere}$$



6th Code: 2D Poisson's Equation

Obtained by adding a source term on the right-hand side of the Laplace's equation

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Discretized form:

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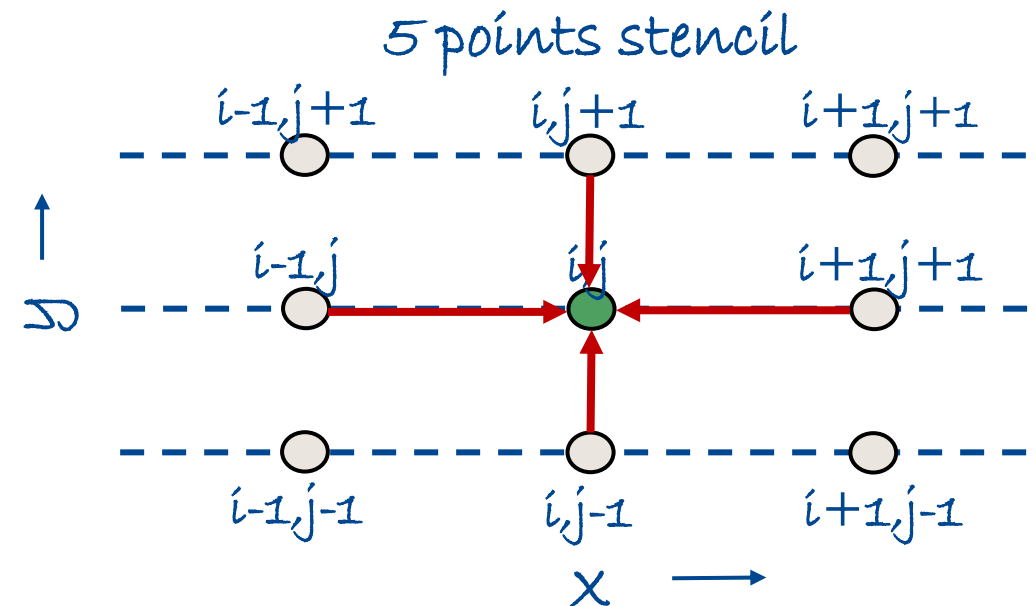
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The iteration will relax the initial spikes!



6th Code: 2D Poisson's Equation

Obtained by adding a source term on the right-hand side of the Laplace's equation

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} = b$$

Poisson's equation act to "relax" the initial sources in the field

Discretized form:

$$\frac{p_{i+1,j}^n - 2p_{i,j}^n + p_{i-1,j}^n}{\Delta x^2} + \frac{p_{i,j+1}^n - 2p_{i,j}^n + p_{i,j-1}^n}{\Delta y^2} = b_{i,j}^n$$

BCs: $p = 0$ at $x = 0, 2$
 $p = 0$ at $y = 0, 2$

$$p_{i,j}^n = \frac{\Delta y^2 (p_{i+1,j}^n + p_{i-1,j}^n) + \Delta x^2 (p_{i,j+1}^n + p_{i,j-1}^n) - b_{i,j}^n \Delta x^2 \Delta y^2}{2(\Delta x^2 + \Delta y^2)}$$

Source term:

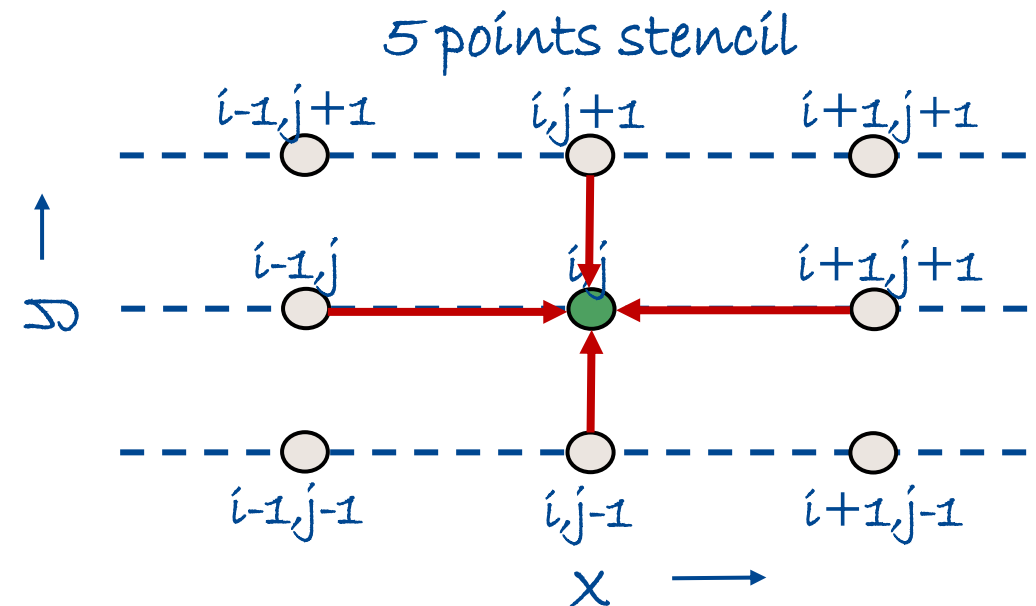
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$$b_{i,j} = 100 \text{ at } i = \frac{3nx}{4}, j = \frac{ny}{4}$$

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The iteration will relax the initial spikes!



6th Code: 2D Poisson's Equation

Obtained by adding a source term on the right-hand side of the Laplace's equation

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} = b$$

Poisson's equation act to "relax" the initial sources in the field

Discretized form:

$$\frac{p_{i+1,j}^n - 2p_{i,j}^n + p_{i-1,j}^n}{\Delta x^2} + \frac{p_{i,j+1}^n - 2p_{i,j}^n + p_{i,j-1}^n}{\Delta y^2} = b_{i,j}^n$$

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$$p_{i,j}^n = \frac{\Delta y^2 (p_{i+1,j}^n + p_{i-1,j}^n) + \Delta x^2 (p_{i,j+1}^n + p_{i,j-1}^n) - b_{i,j}^n \Delta x^2 \Delta y^2}{2(\Delta x^2 + \Delta y^2)}$$

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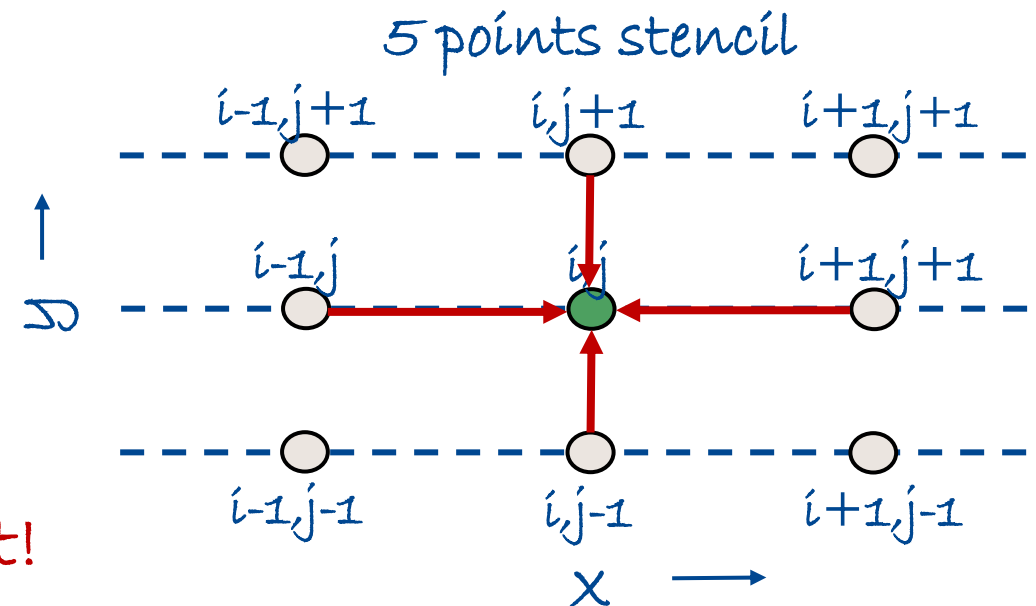
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Let's Code it!





6th Code: 2D Poisson's Equation

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



6th Code: 2D Poisson's Equation

```
import numpy as np
from matplotlib import pyplot, cm
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def plot2D(x,y,p):
    fig = pyplot.figure( figsize=(11,7), dpi=100 )
    ax = fig.gca(projection='3d')
    X, Y = np.meshgrid(x,y)
    surf = ax.plot_surface( X, Y, p[:,], rstride=1, cstride=1, cmap=cm.viridis,
                           linewidth=0, antialiased=False )
    ax.set_xlabel("$x$"); ax.set_xlim(0,2)
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    ax.view_init(30,225)

def poisson2D(p,b,dx,dy,target_norm):
    norm=1; small=1e-8; niter=0
    pn = np.zeros_like(p)
    while norm > target_norm:
        pn = p.copy(); niter+=1
        p[1:-1,1:-1] = ( ( dy**2 * (pn[2:,1:-1] - pn[:-2,1:-1]) +
                           dx**2 * (pn[1:-1,2:] - pn[1:-1,-2]) -
                           dx**2 * dy**2 * b[1:-1,1:-1] ) /
                           (2 * (dx**2 + dy**2)))
        p[0,:] = 0 # p=0 at x=0
        p[-1,:] = 0 # p=0 at x=2
        p[:,0] = 0 # p=0 at y=0
        p[:, -1] = 0 # p=0 at y=2
        norm = (np.sum(np.abs(p)) - np.sum(np.abs(pn)))/(np.sum(np.abs(pn))+small)
    return p
```


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```
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        p[0,:] = 0 # p=0 at x=0
        p[-1,:] = 0 # p=0 at x=2
        p[:,0] = 0 # p=0 at y=0
        p[:,-1] = 0 # p=0 at y=2
        norm = (np.sum(np.abs(p)) - np.sum(np.abs(pn)))/(np.sum(np.abs(pn))+small)
    return p
```

```
nx = 51; ny = 51; dx = 2/(nx-1); dy = 2/(ny-1); nt = 100;
x = np.linspace(0, 2, nx); y = np.linspace(0, 1, ny)
```

6th Code: 2D Poisson's Equation

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

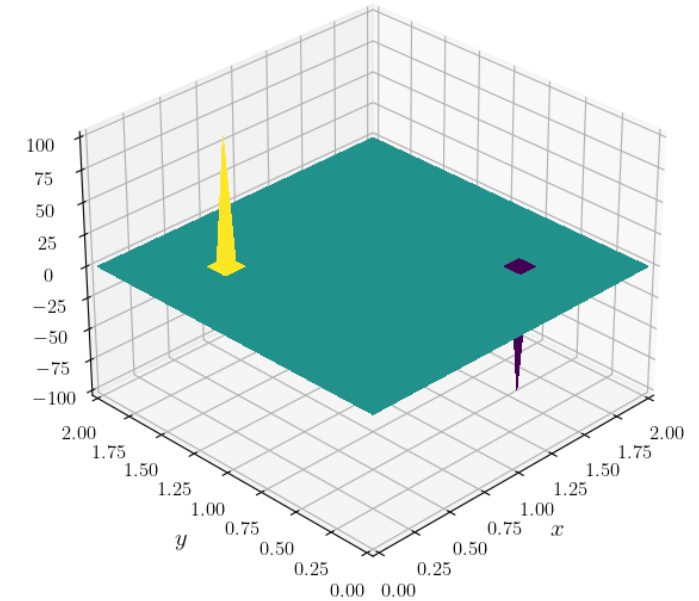
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    ax.set_xlabel("$x$"); ax.set_xlim(0,2)
    ax.set_ylabel("$y$"); ax.set_ylim(0,1)
    ax.view_init(30,225)
```

```
def poisson2D(p,b,dx,dy,target_norm):
    norm=1; small=1e-8; niter=0
    pn = np.zeros_like(p)
    while norm > target_norm:
        pn = p.copy(); niter+=1
        p[1:-1,1:-1] = ( ( dy**2 * (pn[2,1:-1] - pn[:-2,1:-1]) +
                          dx**2 * (pn[1:-1,2:] - pn[1:-1,:-2]) -
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                        (2* (dx**2 + dy**2)))
        p[0,:] = 0 # p=0 at x=0
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        norm = (np.sum(np.abs(p)) - np.sum(np.abs(pn)))/(np.sum(np.abs(pn))+small)
    return p
```

```
p = np.zeros((nx,ny))
b = np.zeros((nx,ny))
```

```
b[int(nx/4), int(3*ny/4)] = -100
b[int(3*nx/4), int(ny/4)] = 100
```

```
plot2D(x,y,p)
plot2D(x,y,b)
```



```
nx = 51; ny = 51; dx = 2/(nx-1); dy = 2/(ny-1); nt = 100;
x = np.linspace(0, 2, nx); y = np.linspace(0, 1, ny)
```

6th Code: 2D Poisson's Equation

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

```
def plot2D(x,y,p):
    fig = pyplot.figure( figsize=(11,7), dpi=100 )
    ax = fig.gca(projection='3d')
    X, Y = np.meshgrid(x,y)
    surf = ax.plot_surface( X, Y, p[:,], rstride=1, cstride=1, cmap=cm.viridis,
                           linewidth=0, antialiased=False )
    ax.set_xlabel("$x$"); ax.set_xlim(0,2)
    ax.set_ylabel("$y$"); ax.set_ylim(0,1)
    ax.view_init(30,225)
```

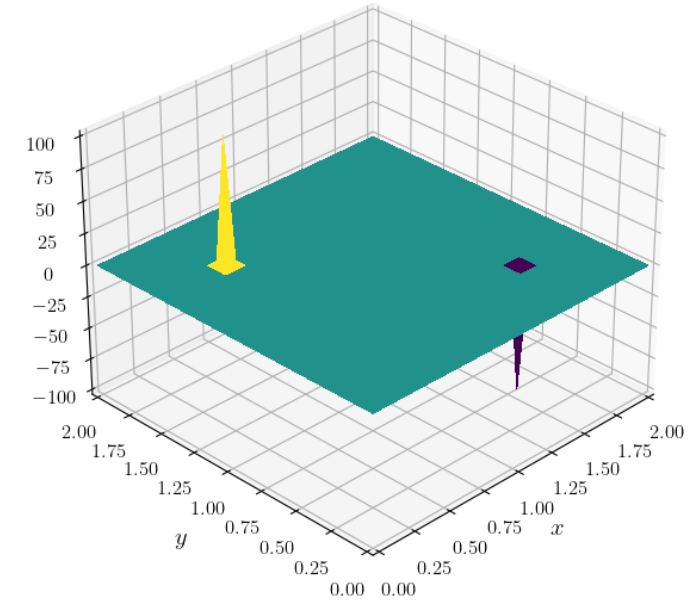
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```

```
plot2D(x,y,p)
plot2D(x,y,b)
```

```
p, niter = poisson2D(p,b,dx,dy,1e-4)
```



```
nx = 51; ny = 51; dx = 2/(nx-1); dy = 2/(ny-1); nt = 100;
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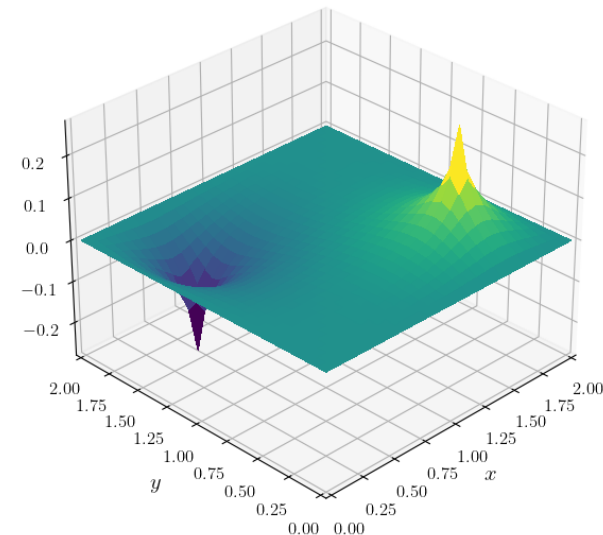
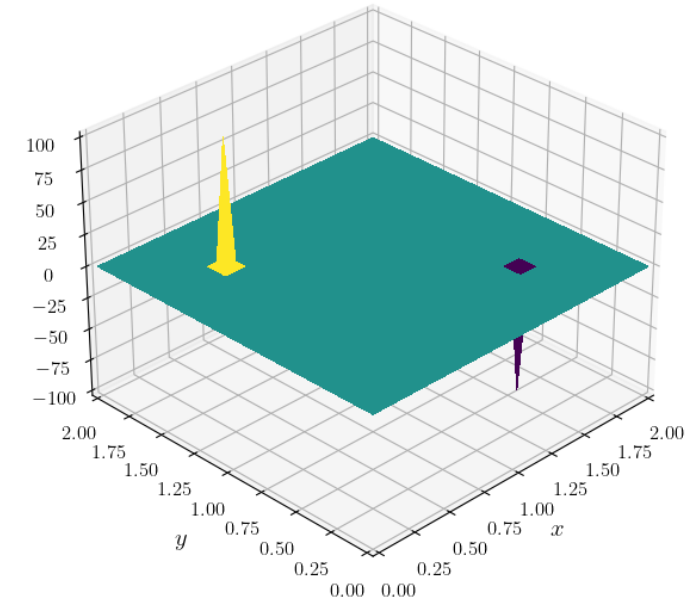
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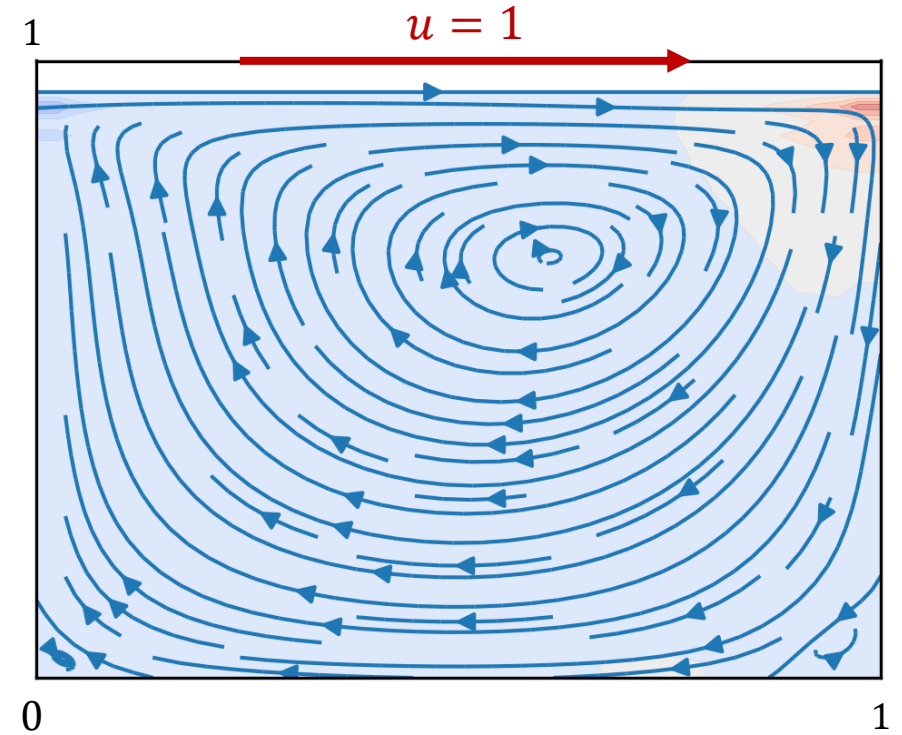
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```
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```

```
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```



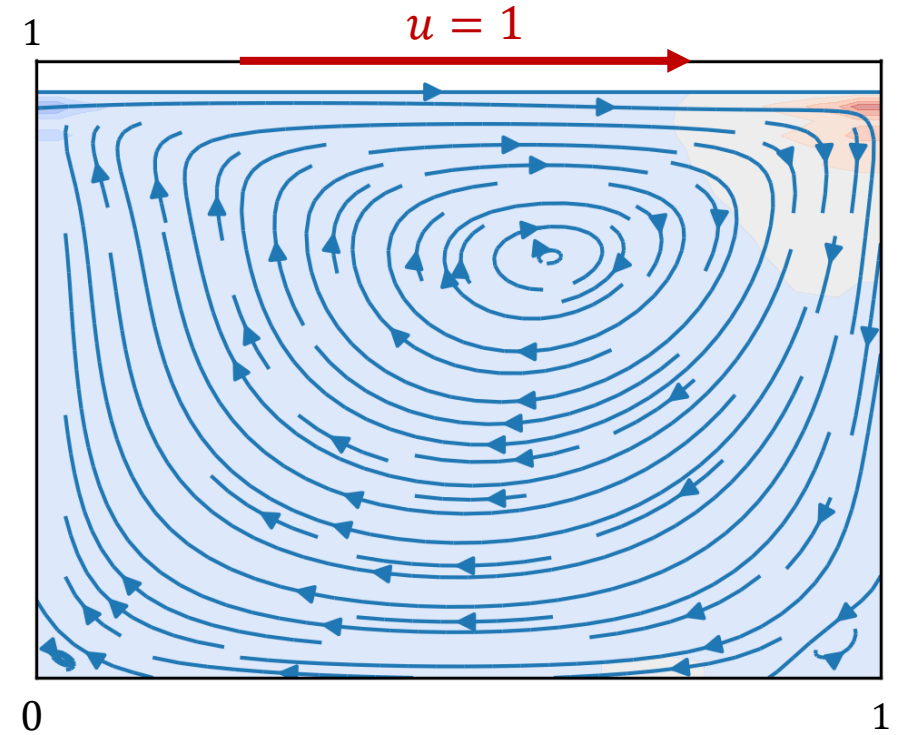
Practical Session: 2D Lid Driven Cavity Flow



Practical Session: 2D Lid Driven Cavity Flow

Continuity: $\nabla \cdot \vec{v} = 0$

Momentum: $\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \vec{v}$



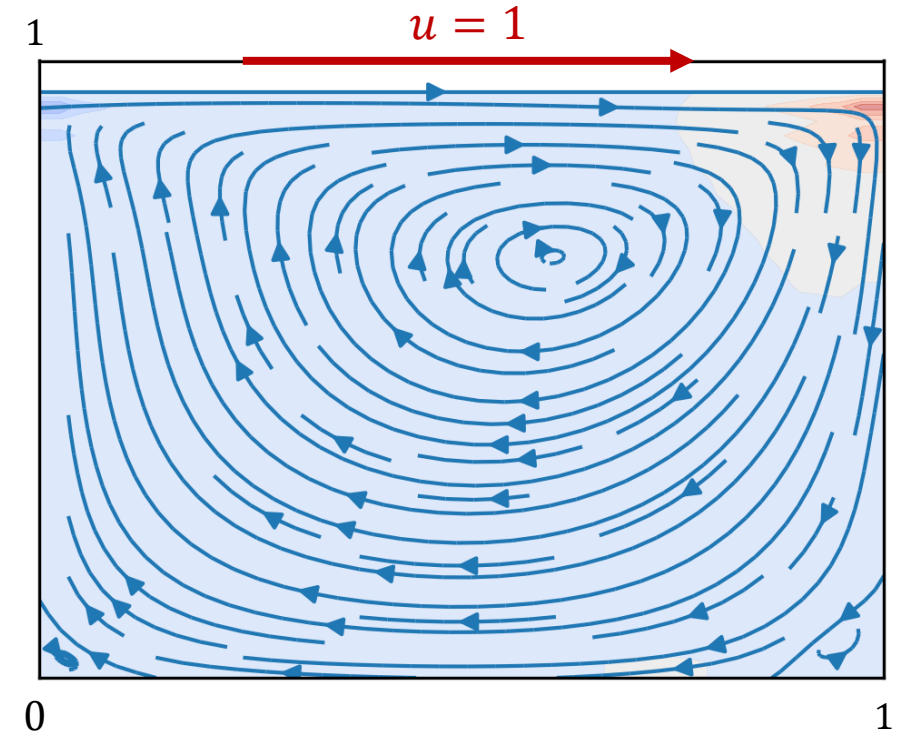
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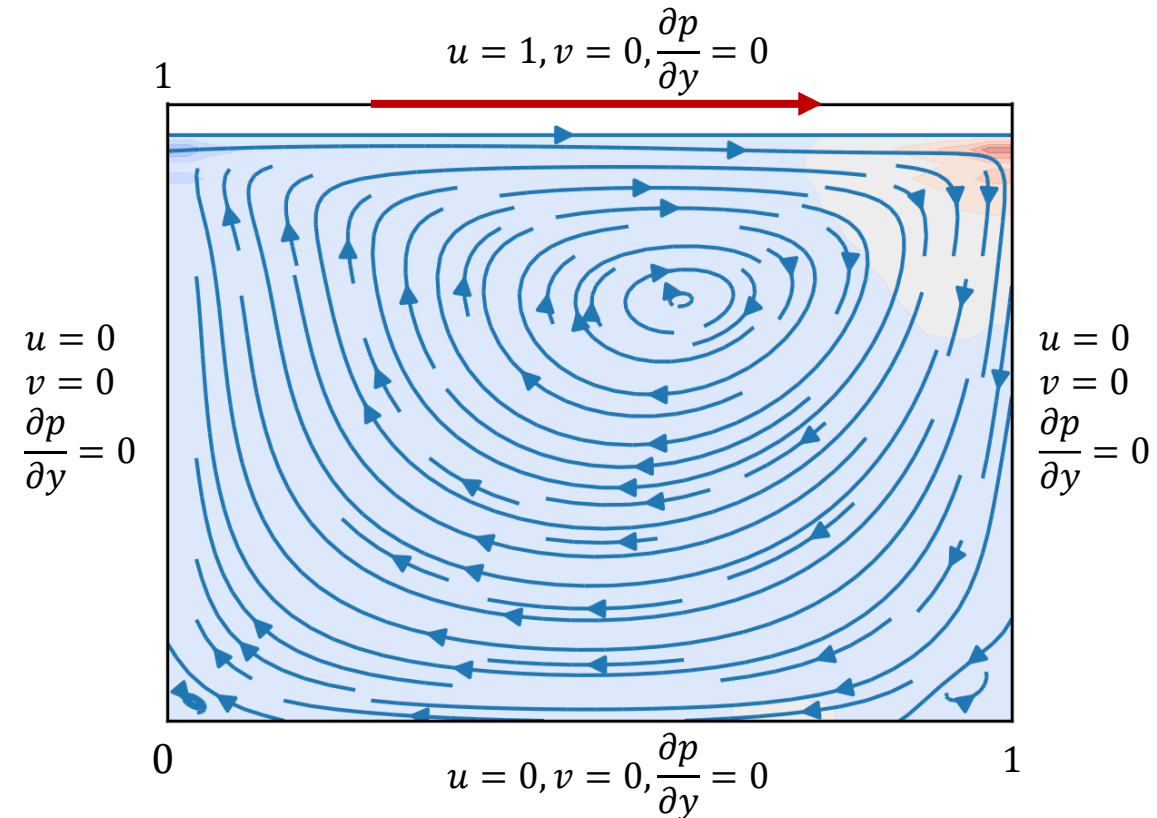
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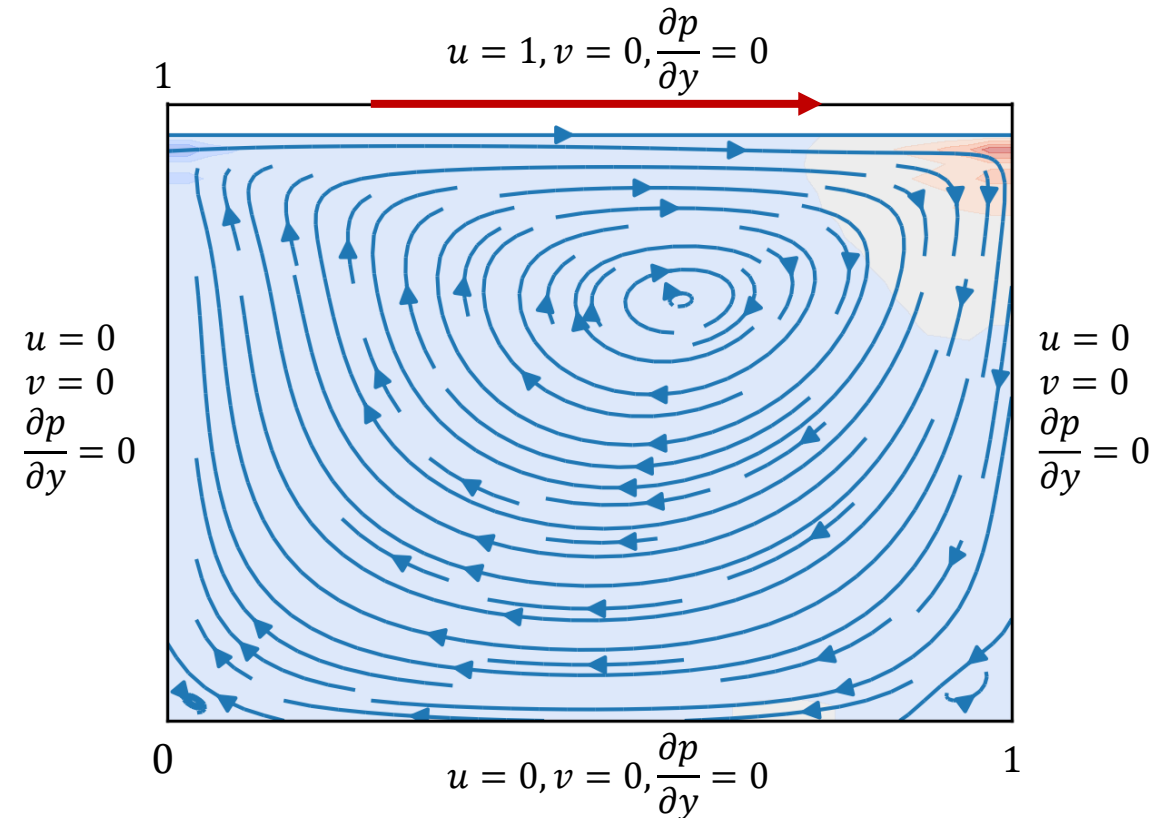
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What about the pressure?



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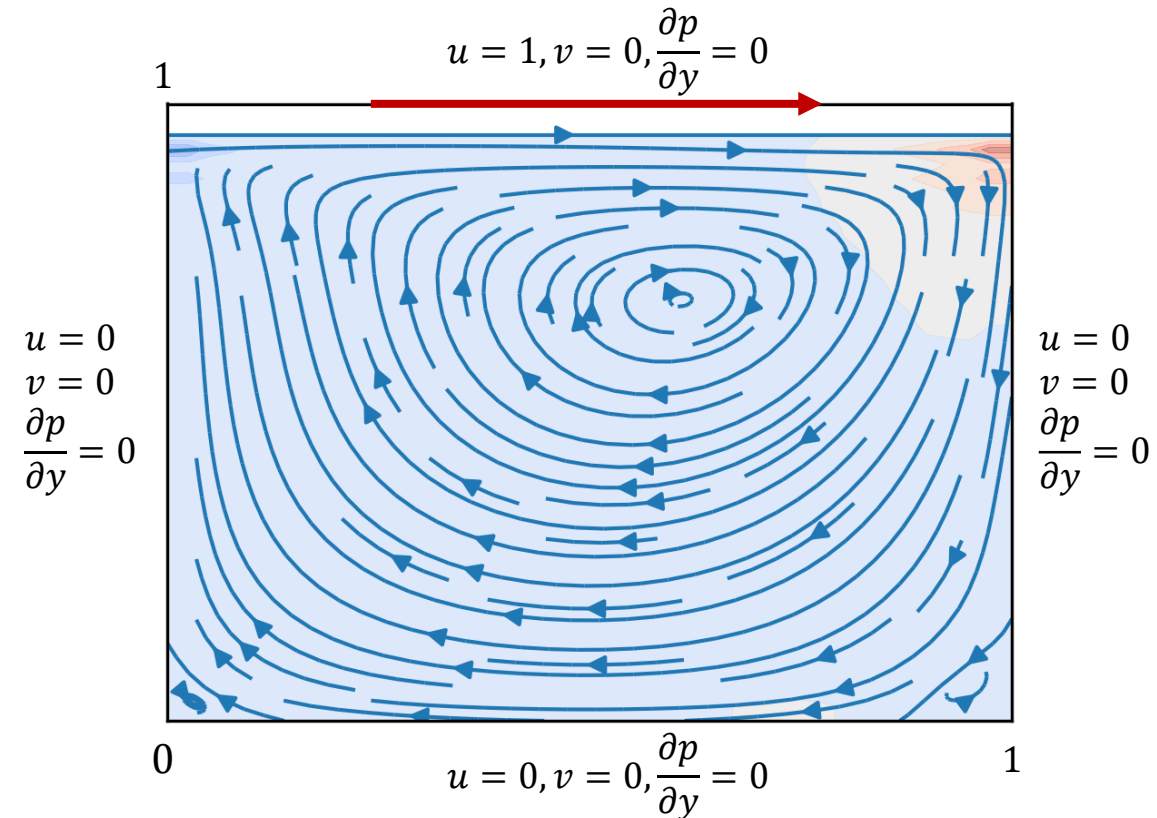
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Recall: The pressure Poisson's Equation

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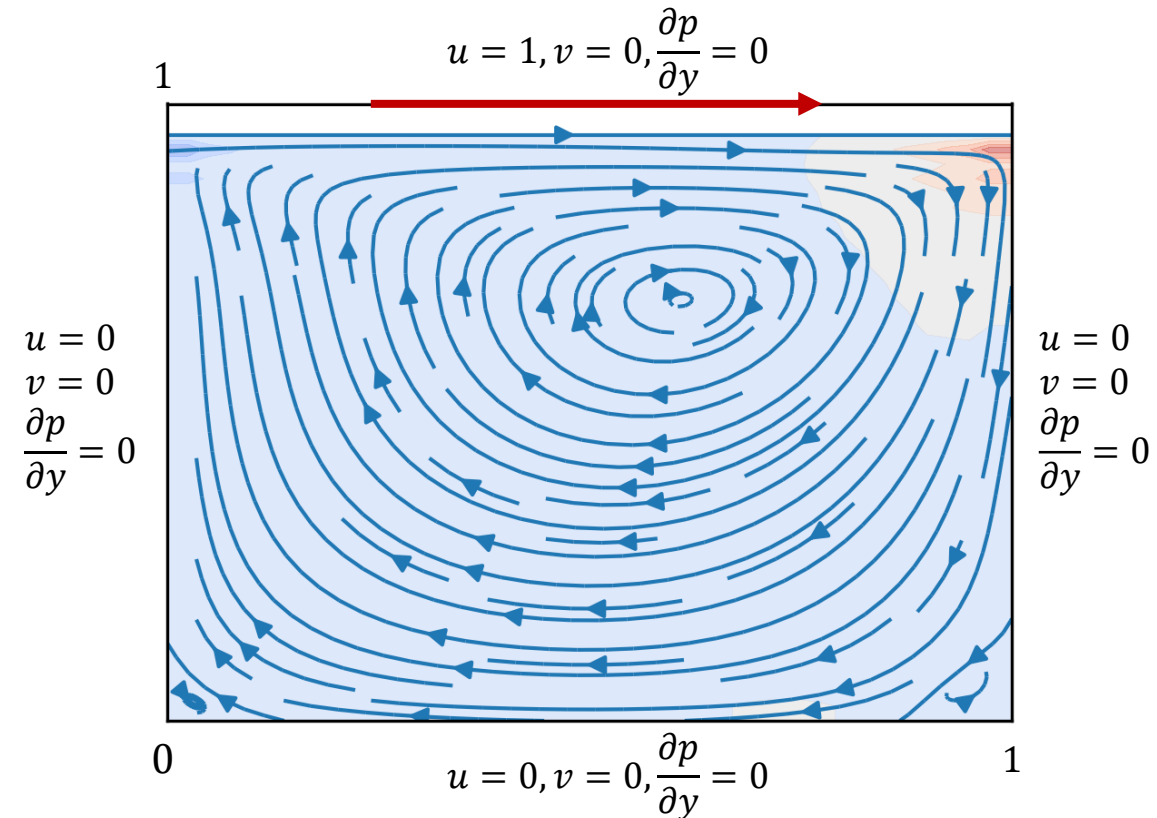
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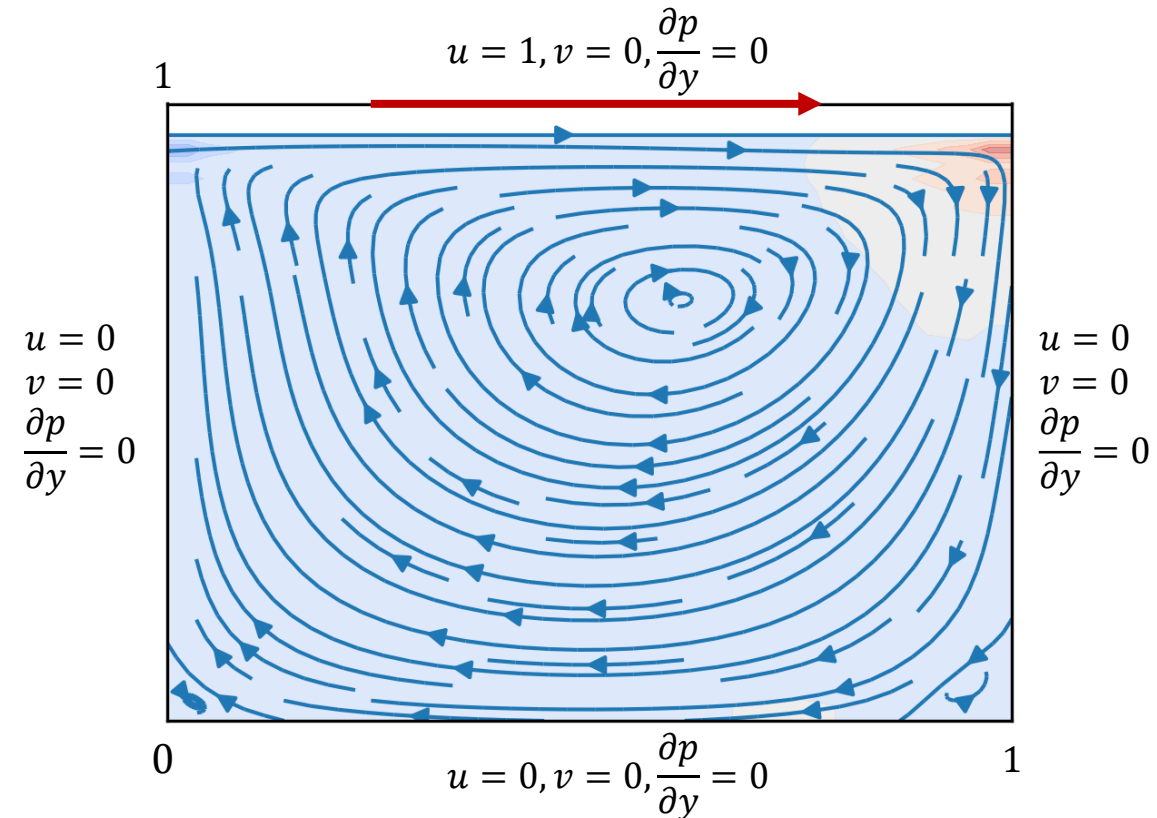
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Now it's your turn to discretize the equations, code it & visualize the results!

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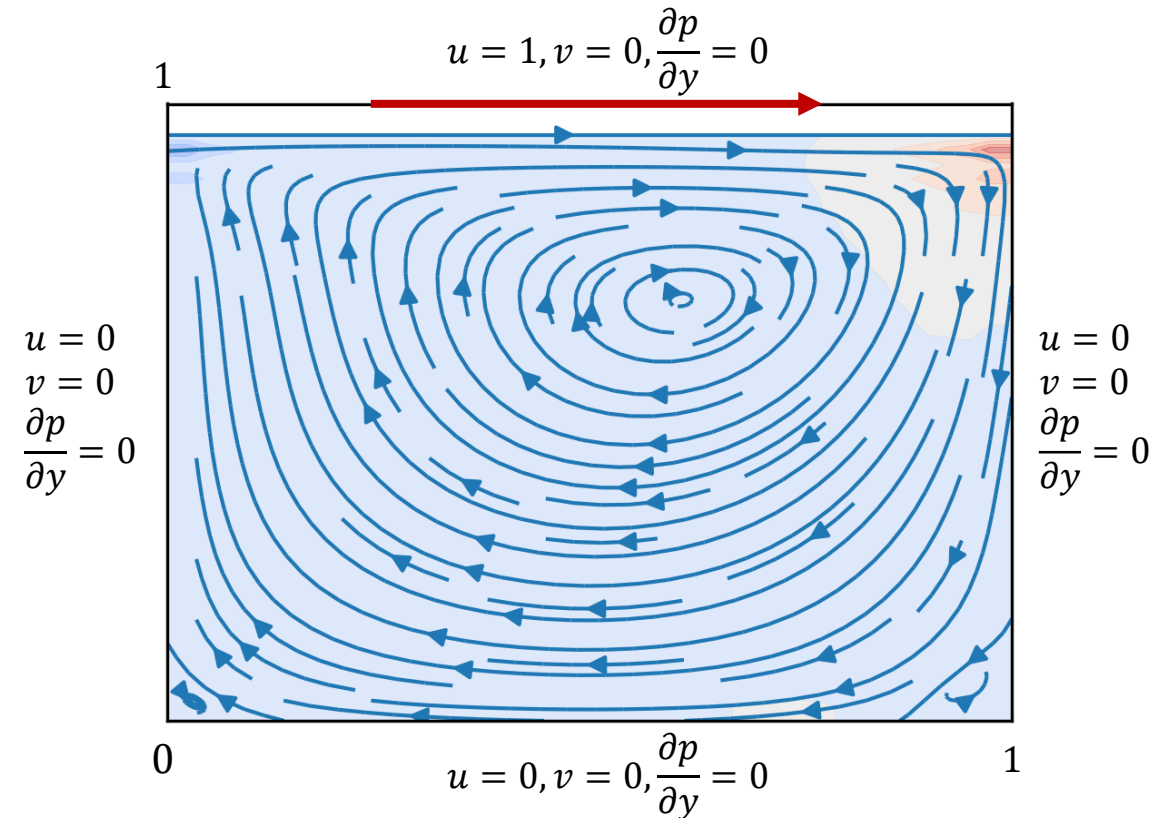
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Good Luck!