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The Continuum

Multi-Scale Modelling IMSE

Part 1
9th November
By Edward Smith

Introduction

Plan for the Continuum Part of the Course

- Where we are in the wider modelling hierarchy
- Understand the Continuum assumption
- Partial differential equations and numerical solutions

Session 1

- More partial differential equations and numerical solutions
- Two dimensional vector fields
- The Navier-Stokes Equation
  - Assumptions that lead to it
  - Key terms and their meaning (with some extensions)
  - Simplifications and solutions

Session 2

- Link to the molecular dynamics equations
- Numerical solutions to the Navier Stokes equation

Session 3

Aims

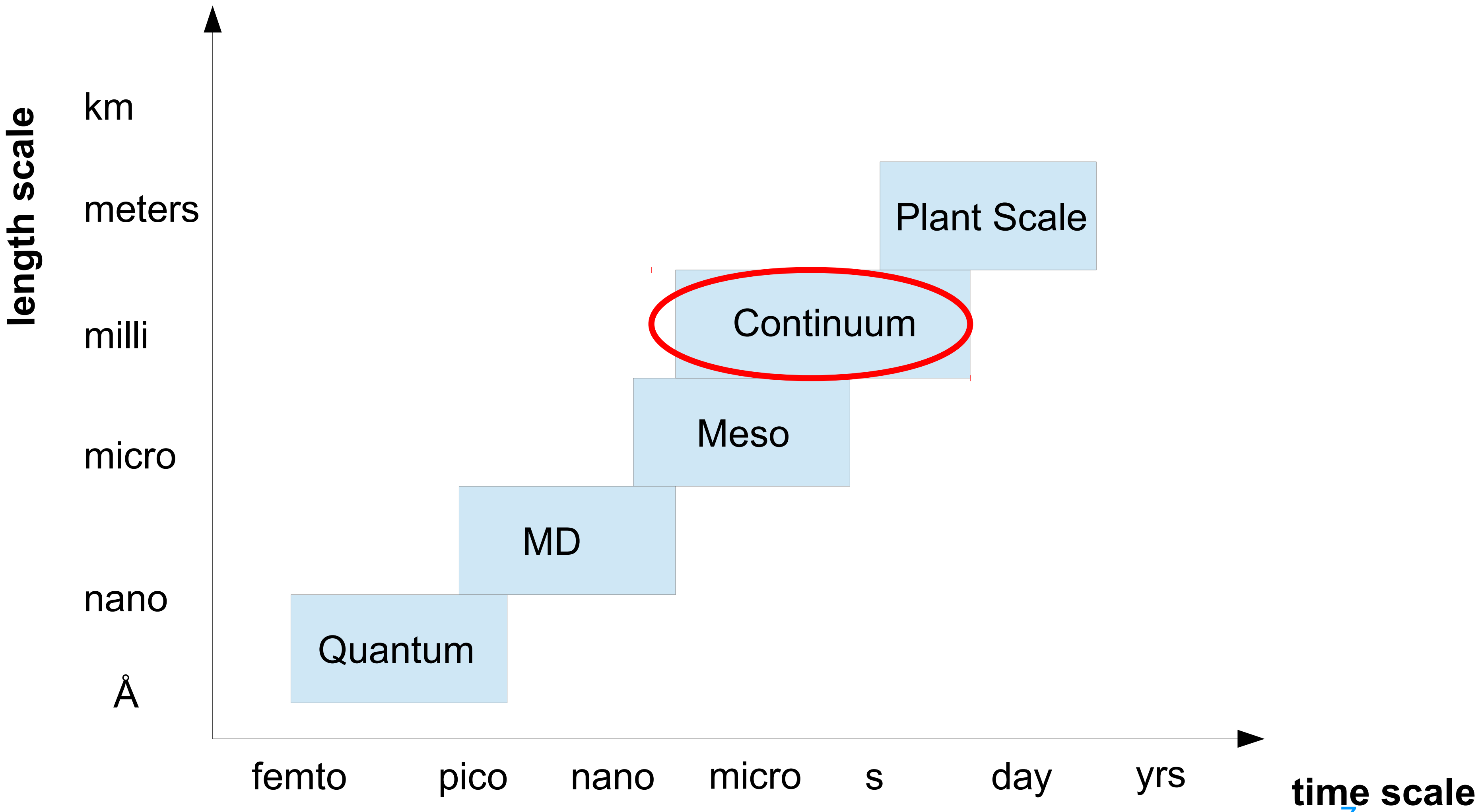
- By the end of the 3 part course you should be able to:
  - State the Continuum assumption, specifically for continuous fields and how this underpins fluid dynamics
  - Understand three dimensional fields, vector calculus and partial differential equations
  - Be able to solve basic differential equations numerically
  - State the Navier-Stokes Equation, key assumptions, the meaning of the terms and how to simplify and solve.
  - Understand how to treat the various terms in a numerical solutions to the Navier-Stokes equation
  - Understand where the continuum modelling fits into the hierarchy and links to the molecular and plant scales

Aims

- By the end of today's session you will have:
  - Seen what the Continuum assumption means and been shown that, crucially, it describes continuous fields
  - An understanding of fields and how to plot them
  - Been introduced to some simple ordinary and partial differential equations
  - Been shown how to solve basic differential equations numerically
  - Tried to solve them using either a programming language of your choice or Excel

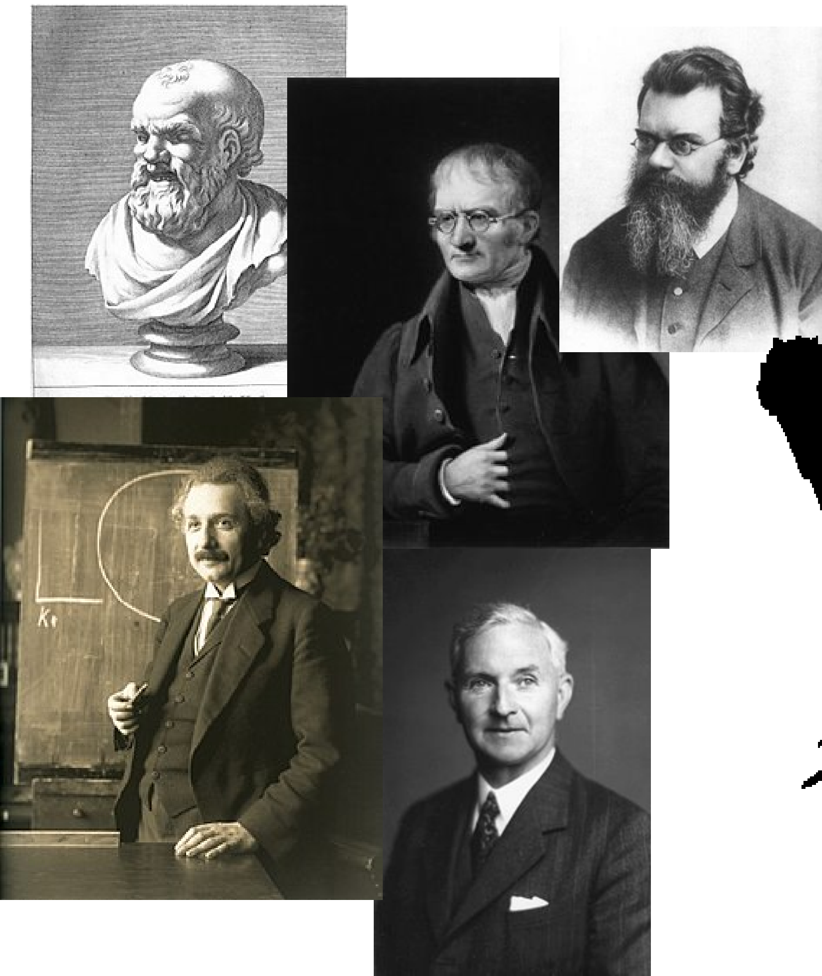
Introduction

Scale Hierarchy



History of the Continuum vs Atomistic

Molecular/Atomistic



VS

Continuum

Video of MD vs Continuum

https://www.youtube.com/watch?v=aQABqOkPXXA

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The Navier-Stokes Equation

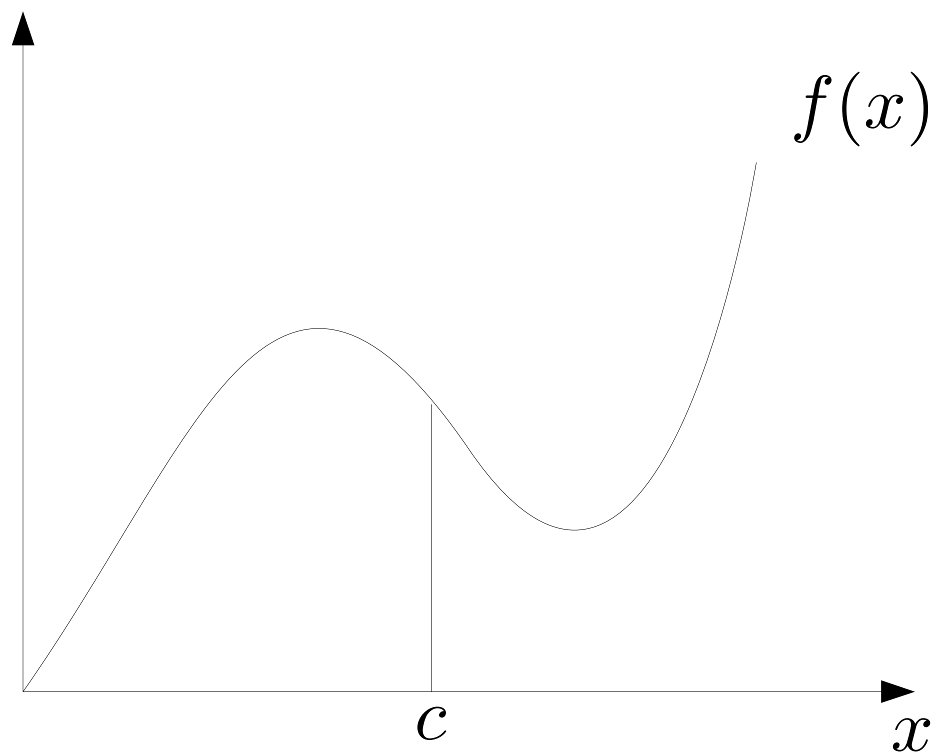
- Describes the flow of single phase Newtonian fluids

$$\underbrace{\frac{\partial \underline{u}}{\partial t}}_{\textbf{Unsteady Term}} + \underbrace{\underline{u} \cdot \underline{\nabla}\, \underline{u}}_{\textbf{Convection Term}} = \underbrace{-\frac{1}{\rho} \underline{\nabla} P}_{\textbf{Pressure Term}} + \underbrace{\nu \nabla^2 \underline{u}}_{\textbf{Diffusion Term}}$$

- Lots of complexity here, a non-linear partial differential equation for velocity and pressure – we'll build up to it
- Apparently impossible to solve directly, complex to solve numerically and not proven to have existence and smoothness (Clay prize with $1,000,000 reward)

The Continuum, Calculus and Differential Equations

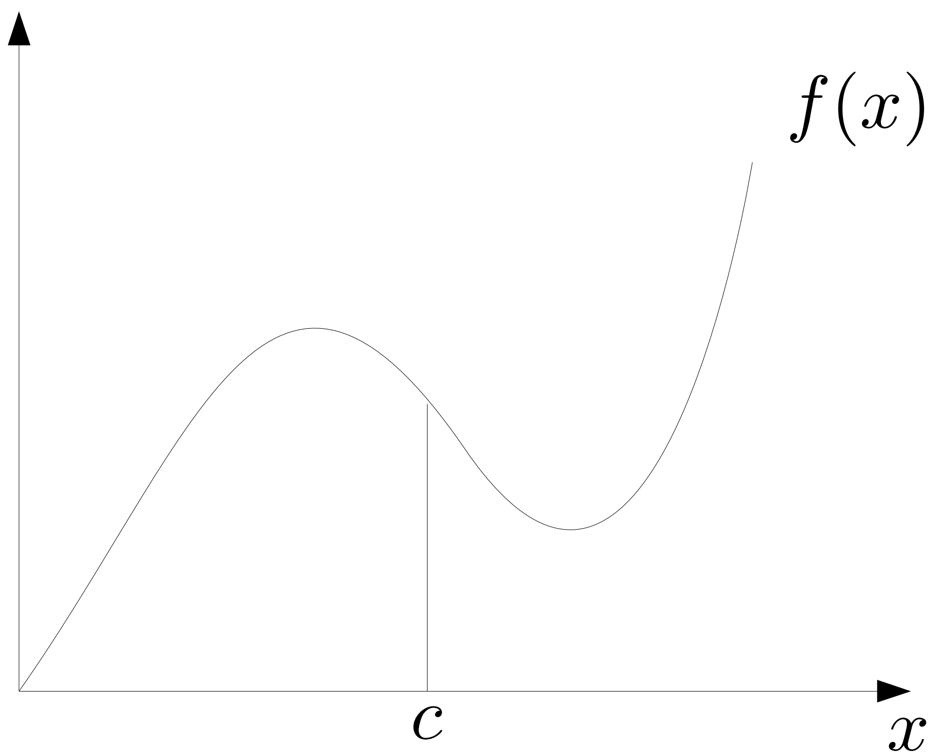
Definition of a Continuous Function



f is continuous if and only if the limit $\lim_{x \to c} f(x)$ exists

Also $\epsilon - \delta$ definition which is more formal.

Definition of a Continuous Function

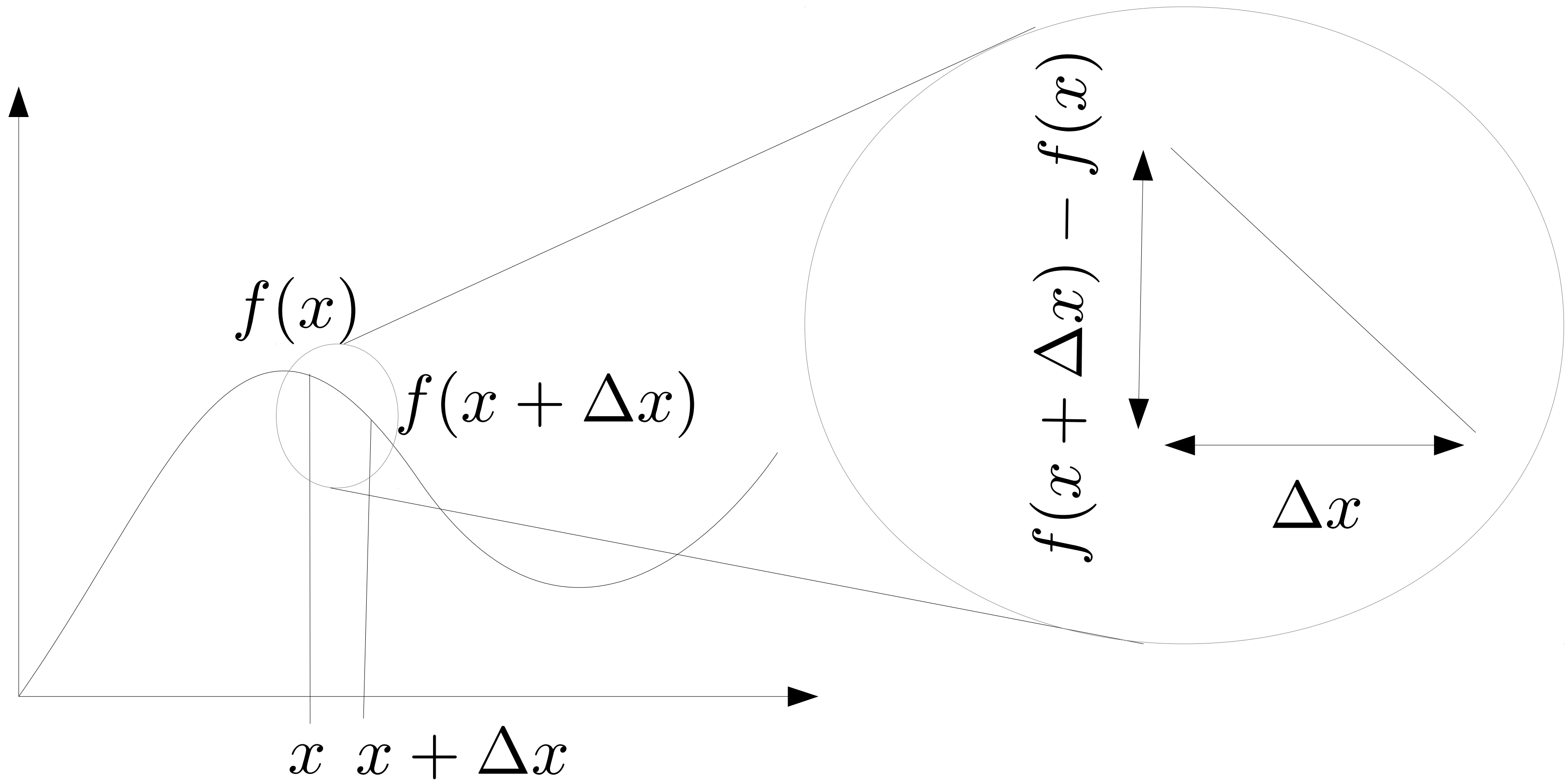


Note the continuum is a definition; essentially an assumption that works very well in most cases (and underpins the majority of applied mathematics)

f is continuous if and only if the limit $\lim_{x \to c} f(x)$ exists

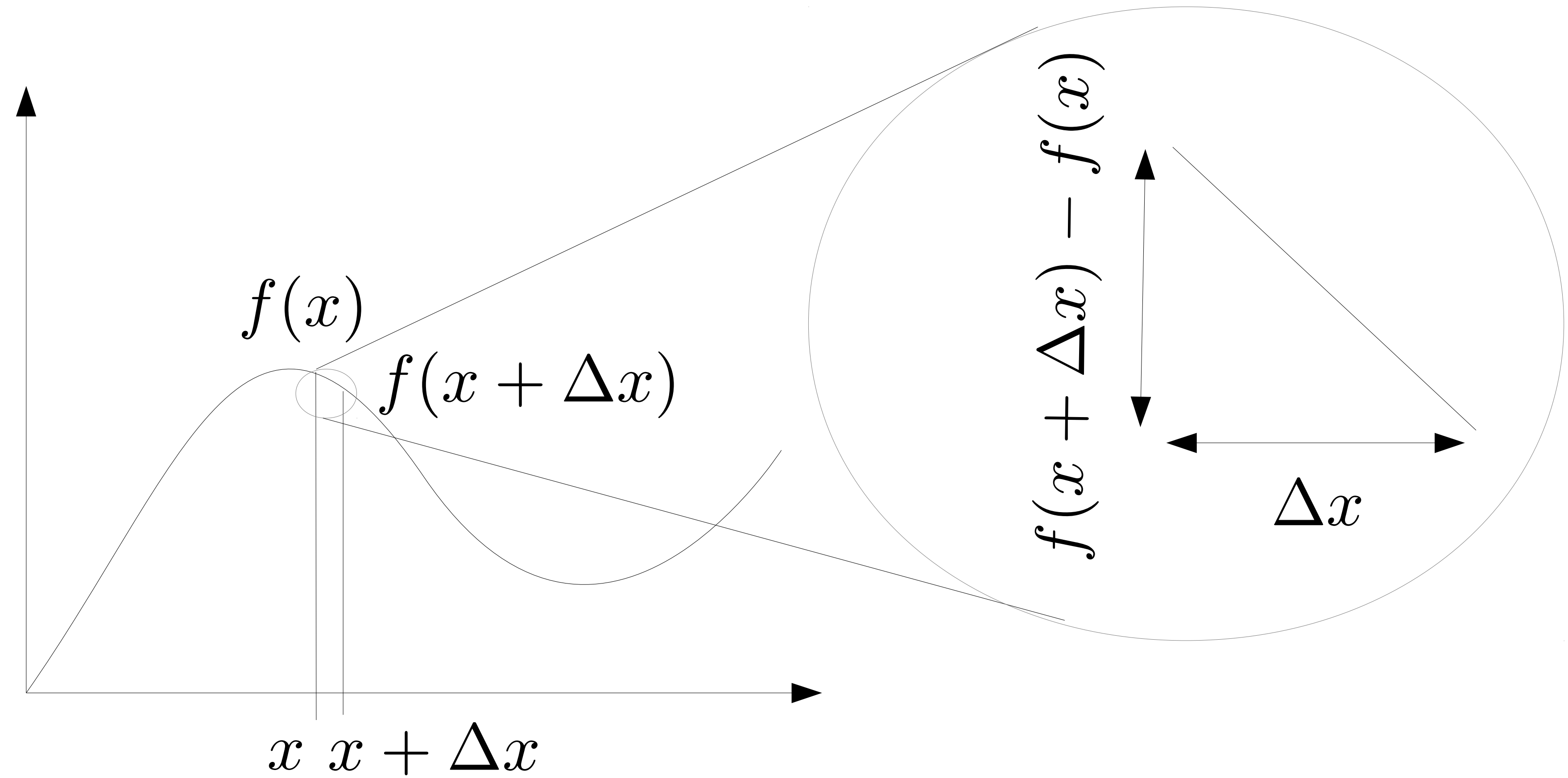
Also $\epsilon - \delta$ definition which is more formal.

Definition of a Derivative



$$\text{Gradient} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

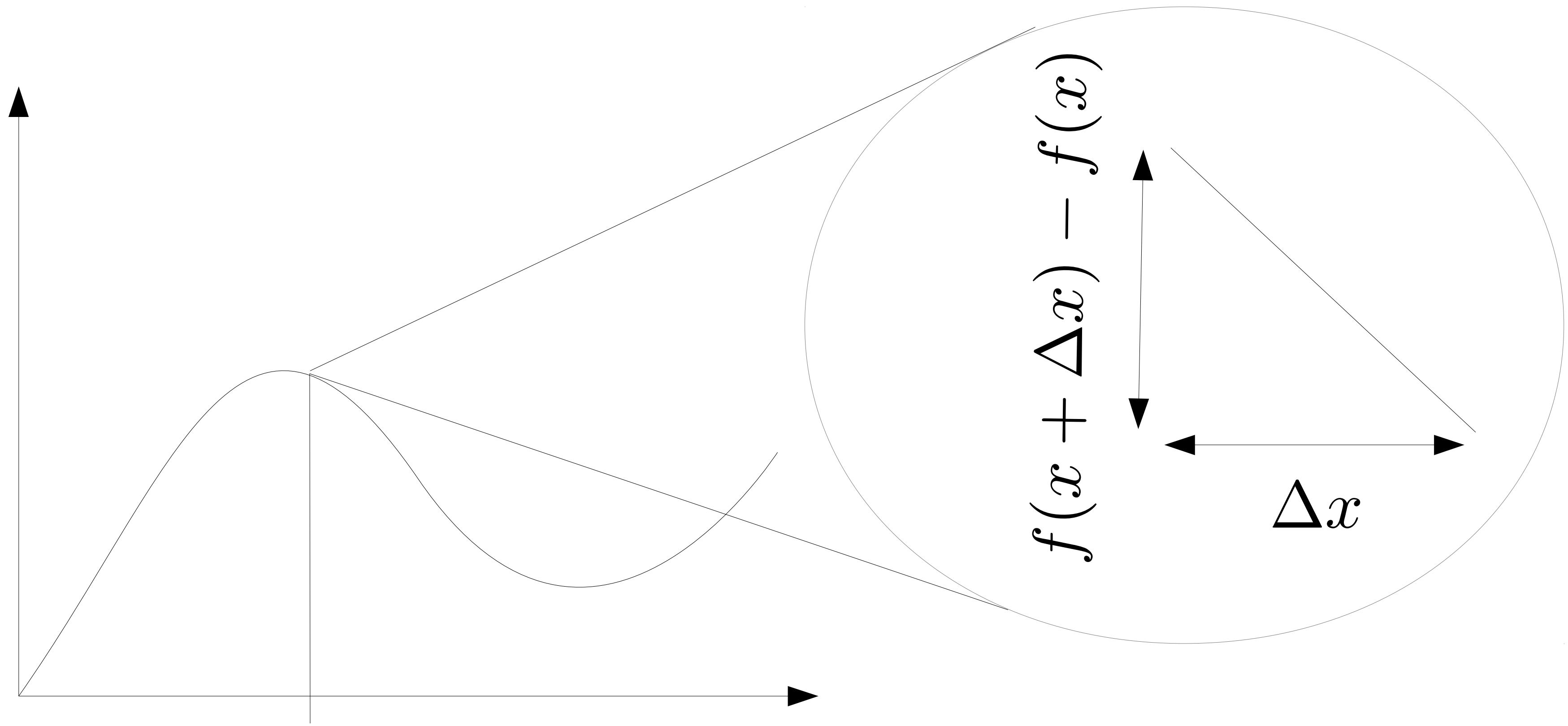
Definition of a Derivative



Better with smaller Δx

$$\text{Gradient} \approx \frac{f(x+\Delta x)-f(x)}{\Delta x}$$

Definition of a Derivative



Exact in Limit $\Delta x \to 0$ $$\frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

Differential Equations

- Equations which include derivatives are differential equations, e.g.

$$\frac{df}{dx} = 0 \qquad \frac{df}{dx} = ax + b \qquad \frac{d^2 f}{dx^2} = 5$$

- These are the same as any other equation, for example the equation for a line or Newton's law

$$y = mx + c \qquad F = ma$$

- Which can also be written as differential equations

$$y = \frac{dy}{dx}x + c \qquad F = m\frac{d^2 x}{dt^2}$$

Differential Equations

- Equations which include derivatives are differential equations, e.g.

$$\frac{d^3 f}{dx^3} + \frac{df}{dx} = 9 \qquad \frac{d^2 f}{dx^2} = 0 \qquad \frac{df}{dx} + x = 0$$

- Order of equation is highest derivative, here 3, 2 and 1

- Equations can be linear or non-linear. Roughly speaking, any equation which contains a product of unknown function or it's derivatives (here f) is non-linear, e.g.

$$f\frac{d^2 f}{dx^2} + x\frac{df}{dx} = 0 \qquad \frac{d^4 f}{dx^4} + f^2 = 0 \qquad \left(\frac{df}{dx}\right)^2 + x^2 = 0$$

Differential Equations

- Differential equations are useful because they describe physics in the continuum, for example the Wave Equation

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

- The Advection-Diffusion Equation (for some chemical concentration C, diffusing with coefficient D

$$\frac{\partial C}{\partial t} = \boldsymbol{\nabla} \cdot (D \boldsymbol{\nabla} C) - \boldsymbol{\nabla} \cdot (\underline{u} C)$$

- Even Newton's Law, which is continuous in time

$$m \frac{dx^2}{dt^2} = F$$

Solving Differential Equations

- Some differential equations, especially if they are linear, can be solved exactly. For example:

$$\frac{df}{dx} = a \qquad\qquad f(x) = ax + C_1$$

- This is integrated to give f as a function of x with an arbitrary constant of integration. Also for second order equations,

$$\frac{d^2 f}{dx^2} = b \qquad\qquad \frac{df}{dx} = bx + C_2$$

$$f(x) = bx^2 + C_2 x + C_3$$

- Most differential equations are too complex to solve directly, research typically focuses on numerical solutions

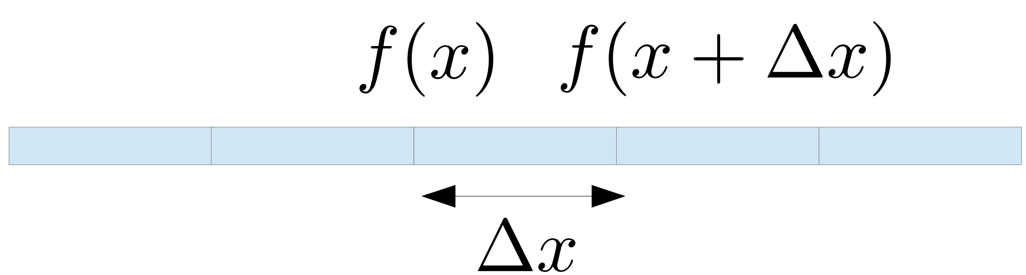
Numerical Solution to Differential Equations

- Instead we solve numerically, consider the definition of the derivative

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

If we make delta x small we can approximate the derivative by taking two points which are arbitrarily close

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



Numerical Solution to Differential Equations

- First order derivatives

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

- Second order derivatives

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

- We can introduce short-hand notation for this

$$\frac{f(x+\Delta x) - f(x)}{\Delta x} \equiv \frac{f_{i+1} - f_i}{\Delta x}$$

$$\frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{(\Delta x)^2} \equiv \frac{f_{i+1} - 2f_i + f_{i-1}}{(\Delta x)^2}$$

Numerical Solution to Differential Equations

- First order derivatives

$$\frac{df}{dx} \approx \frac{f_{i+1} - f_i}{\Delta x}$$

- Second order derivatives

$$\frac{d^2 f}{dx^2} \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{(\Delta x)^2}$$

- How to write this as code, as an example we consider

for $\frac{df}{dx} = a$ and use $\frac{df}{dx} \approx \frac{f_{i+1} - f_i}{\Delta x}$

and rearrange to get i+1 value,

$$f_{i+1} = f_i + a\Delta x \longrightarrow$$

```
f[i+1] = f[i] + a*dx
```

Numerical Solution to Differential Equations

- First order derivatives

$$\frac{df}{dx} \approx \frac{f_{i+1} - f_i}{\Delta x}$$

- Second order derivatives

$$\frac{d^2 f}{dx^2} \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{(\Delta x)^2}$$

- How to write this as code (rearranged to get i+1 value)

$$\frac{df}{dx} = a$$

```
f[i+1] = f[i] + a*dx
```

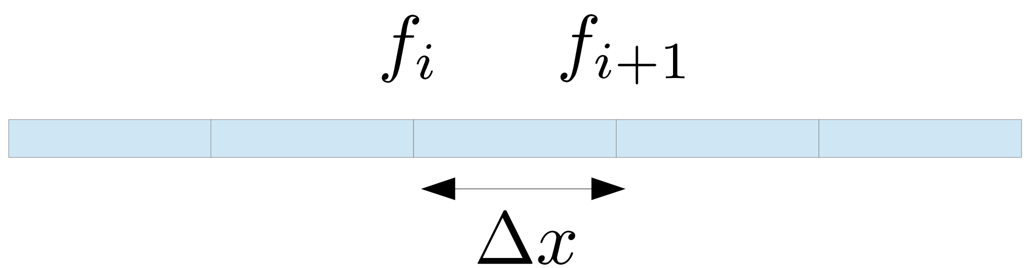
$$\frac{d^2 f}{dx^2} = b$$

```
f[i+1] = 2*f[i] - f[i-1] + b*dx**2
```

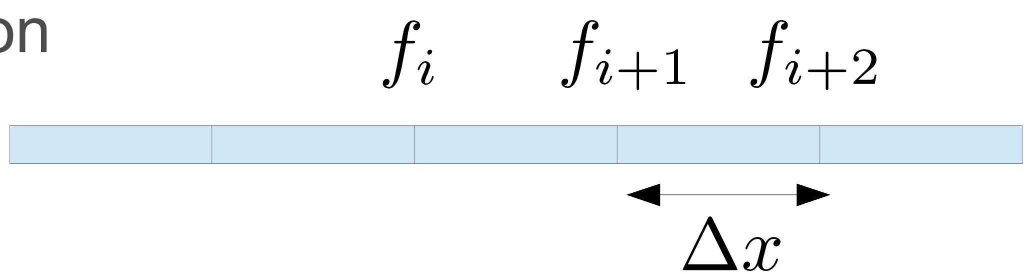
Numerical Solution to Differential Equations

- So if we know the value at f_i, we can get the value at f_{i+1} a small distance, delta x, away

$$\frac{df}{dx} = a \qquad f_{i+1} = f_i + a\Delta x$$



- Once we know the value at f_{i+1}, we can get the value at at f_{i+2}, and so on



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Python vs MATLAB

```
%MATLAB
clear all
close all

x = linspace(0,2*pi,100);
y = sin(x);
z = cos(x);
plot(x,y,'-r');
hold all
plot(x,z,'-b')
```

```
#python
from numpy import *
from matplotlib.pyplot import *

x = linspace(0,2*pi,100)
y = sin(x)
z = cos(x)
plot(x,y,'-r')
plot(x,z,'-b')
show()
```

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Python vs MATLAB

- Loop “for i in range(1, Nsteps-1)” where range(1, Nsteps-1) replace 1:Nsteps in MATLAB's “for i=1:Nsteps”
- Python uses zero indexing (arrays start from 0)
- Square brackets to access array elements, normal brackets for functions (e.g. range function here)
- Indentation used to define scope (four spaces here) no end statements needed after loop

```
for i in range(1,Nsteps-1):
    #Comment with hash
    f[i+1] = 2.*f[i] - f[i-1] + dt**2 * F
plot(x, 'bo')
show()
```

- Plots added to figure will only appear when show() called

Questions 1

1) Use the definition of the derivative $\frac{df}{dx} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$ to calculate $f(x) = x^3$

2) Identify order of the following. Which are linear?

$a)\ \frac{d^3y}{dx^3} + (\frac{dy}{dx})^2 = 4 \qquad b)\ x^2\frac{d^2y}{dx^2} + 3(y-x) = 5x\frac{dy}{dx} \qquad c)\ \frac{dy}{dx} = \frac{y-x}{y+x}$

3) Integrate Newton's Law for constant acceleration,

$$\frac{dx^2}{dt^2} = -g \text{ with } x = 0 \text{ and } \frac{dx}{dt} = v_0 \text{ at } t = 0$$

using initial conditions to replace integration constants. Solve numerically on a computer and compare results

4) Now solve $\frac{dx^2}{dt^2} = \left(\frac{1}{x} - g\right)$ with varying initial conditions. What do you notice?

Fields and Partial Differential Equations

Continuum Fields

- We use Newton's law assuming continuity in time and position (even in a discrete molecular system)
- The Continuum hypothesis refers to the continuous nature of fields in space. These are 2D or 3D continuous functions which evolve in time
- Assumes that we have so many particles it is a continuum.
- In practice, one meter cube of air has 10^{25} molecules so works very well
- Although this also works down to smaller scales than would be expected...

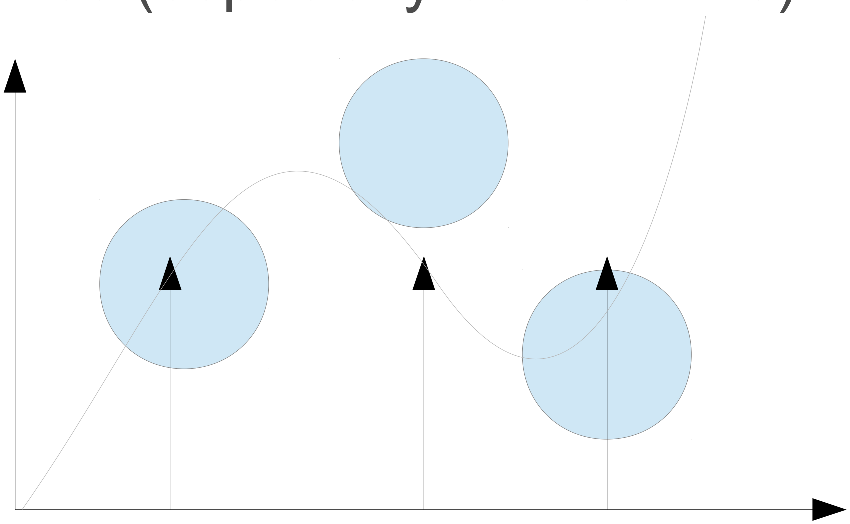
Continuum Fields

f is continuous if and only if the limit $\lim_{x \to c} f(x)$ exists

- When is this not true?
  - When the Molecular nature becomes apparent
  - Extreme events like shock waves
  - Discontinuities or near boundaries (especially contact line)
  - Fractal systems?
- How do we tell if valid
  - Knudsen number for gases

$$Kn = \frac{\lambda}{L}$$

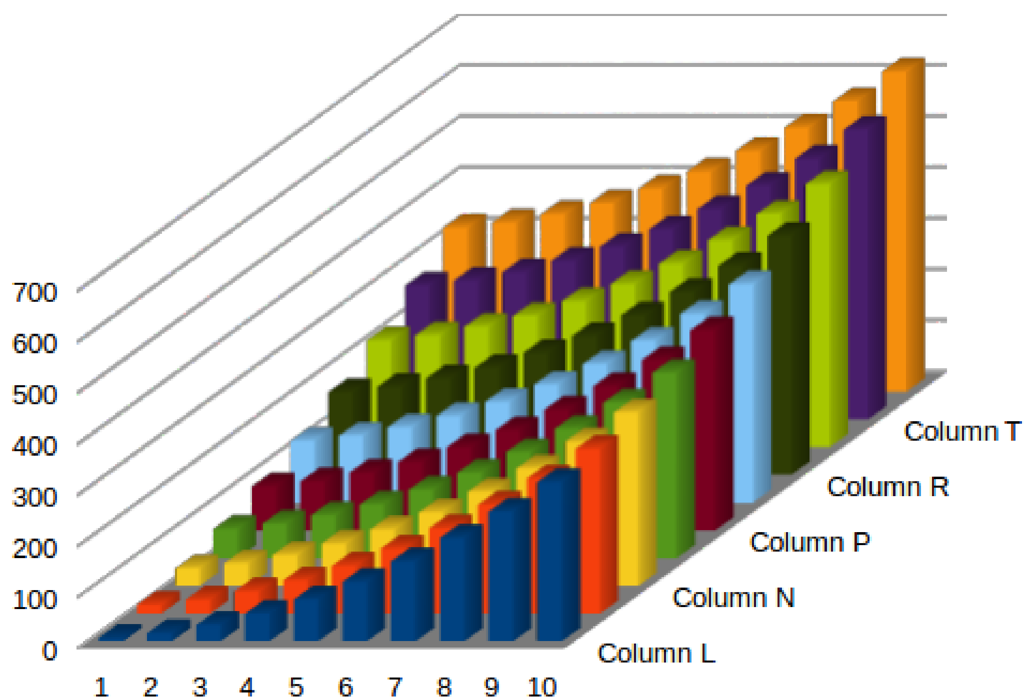
  - No Similar metric for dense fluids (most cases of interest)



Example of a Field

- Consider an example 2D field described by an x-y polynomial

$$f(x, y) = ax^2 + bx + cy^2 + dy + exy + f$$



- Consider a grid of x and y values

$$f = f(x, y)$$

- We plot a bar at each x or y location with the value there

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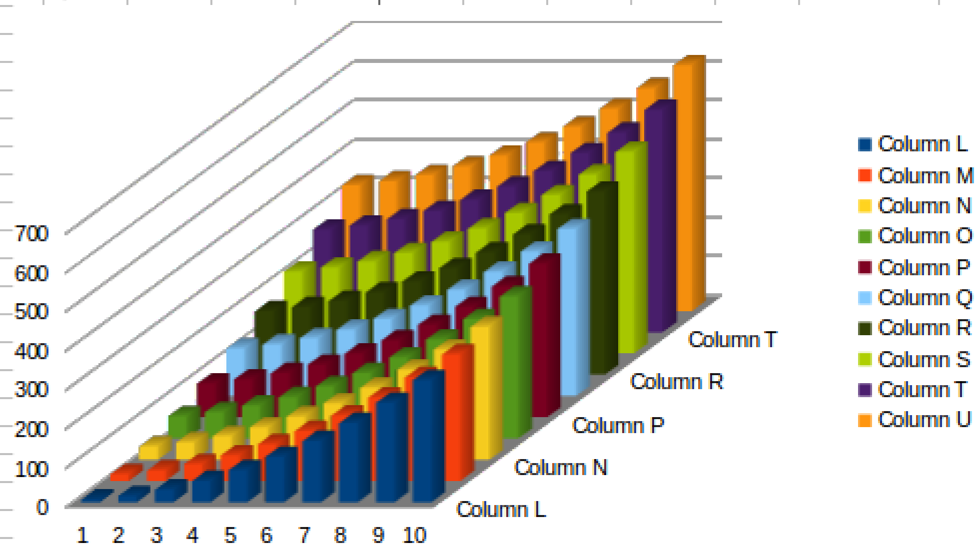
Example of a Field

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1	x											f										
2	1	2	3	4	5	6	7	8	9	10		7	18	35	58	87	122	163	210	263	322	
3	1	2	3	4	5	6	7	8	9	10		17	28	45	68	97	132	173	220	273	332	
4	1	2	3	4	5	6	7	8	9	10		33	44	61	84	113	148	189	236	289	348	
5	1	2	3	4	5	6	7	8	9	10		55	66	83	106	135	170	211	258	311	370	
6	1	2	3	4	5	6	7	8	9	10		83	94	111	134	163	198	239	286	339	398	
7	1	2	3	4	5	6	7	8	9	10		117	128	145	168	197	232	273	320	373	432	
8	1	2	3	4	5	6	7	8	9	10		157	168	185	208	237	272	313	360	413	472	
9	1	2	3	4	5	6	7	8	9	10		203	214	231	254	283	318	359	406	459	518	
10	1	2	3	4	5	6	7	8	9	10		255	266	283	306	335	370	411	458	511	570	
11	1	2	3	4	5	6	7	8	9	10		313	324	341	364	393	428	469	516	569	628	
12																						
13	y																					
14	1	1	1	1	1	1	1	1	1	1												
15	2	2	2	2	2	2	2	2	2	2												
16	3	3	3	3	3	3	3	3	3	3												
17	4	4	4	4	4	4	4	4	4	4												
18	5	5	5	5	5	5	5	5	5	5												
19	6	6	6	6	6	6	6	6	6	6												
20	7	7	7	7	7	7	7	7	7	7												
21	8	8	8	8	8	8	8	8	8	8												
22	9	9	9	9	9	9	9	9	9	9												
23	10	10	10	10	10	10	10	10	10	10												
24																						
25		coefficients																				
26		a	3																			
27		b	2																			
28		c	3																			
29		d	1																			
30		e	0																			
31		f	-2																			
32																						
33																						
34																						

$$f(x,y) = ax^2 + bx + cy^2 + dy + exy + f$$



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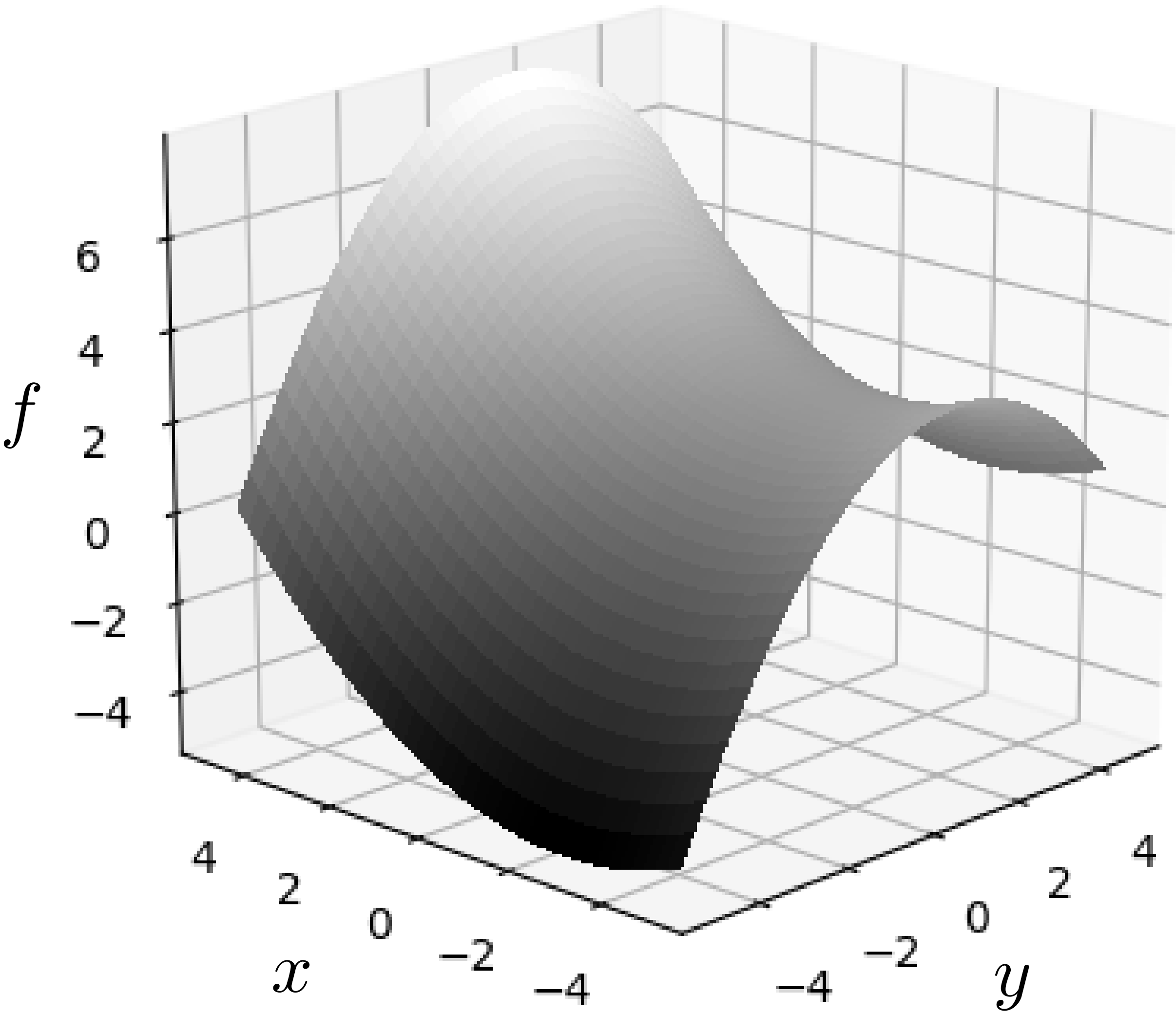
Two Dimensions Fields (3D plot)



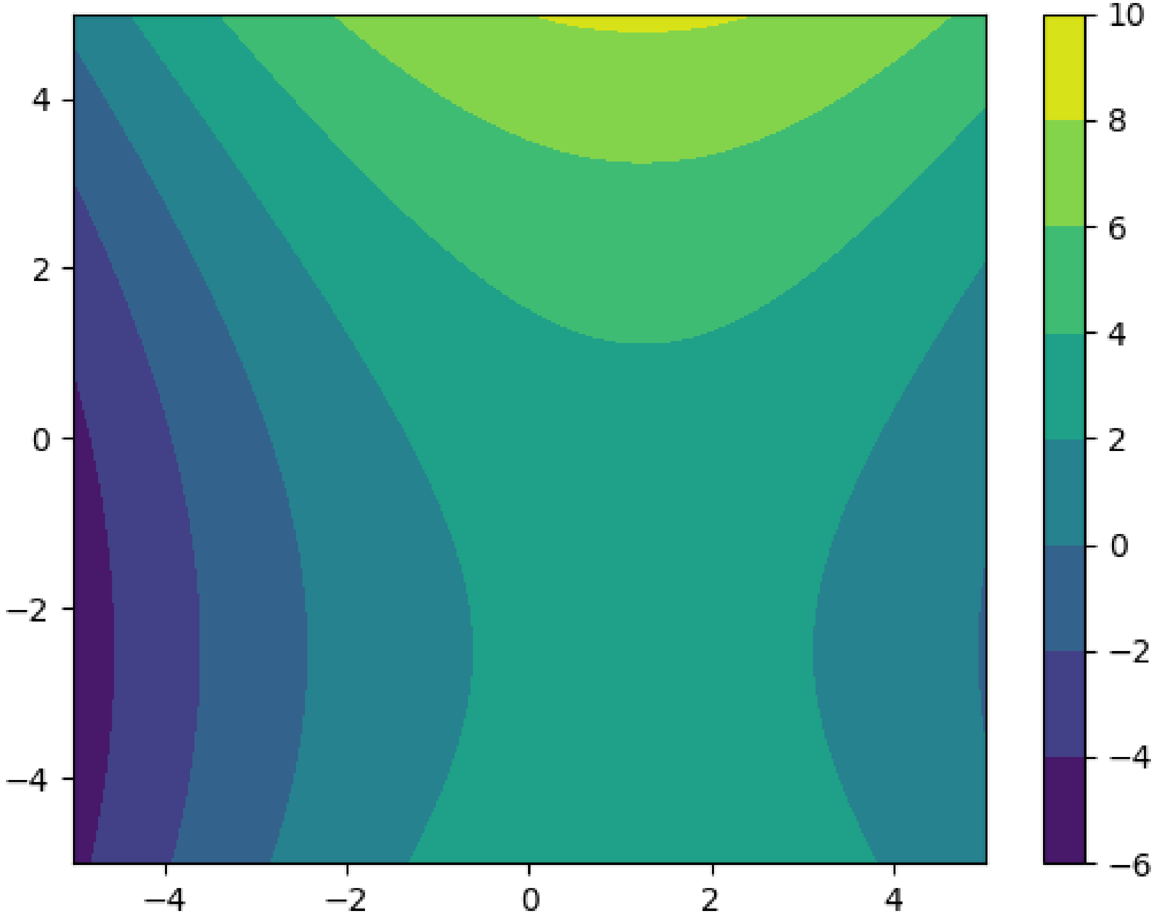
- Limit is a continuous function
- Here a function of two variables

$$f = f(x, y)$$

- As we move in either x or y direction the value of f changes

Two Dimensions Fields (2D plot)

- Contour plot



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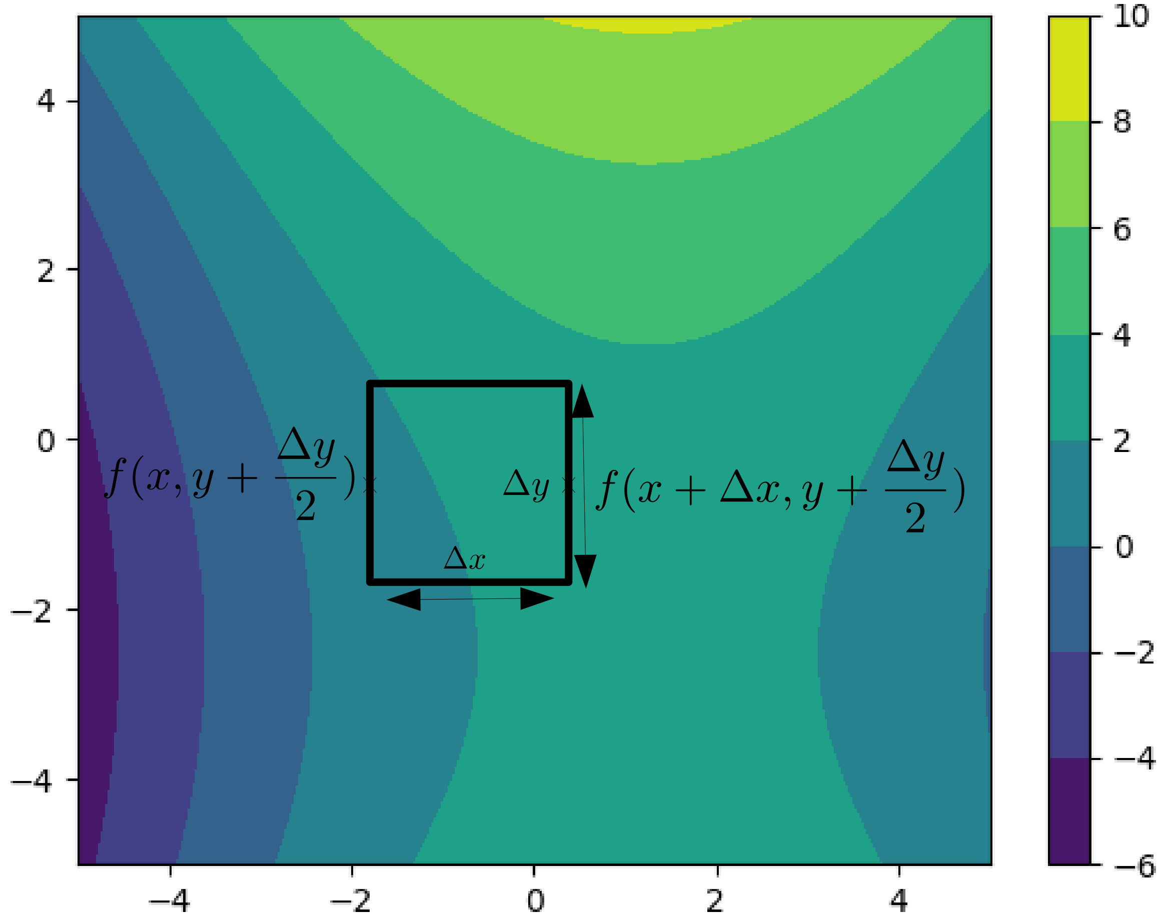
Two Dimensions Fields (2D plot)

- Contour plot



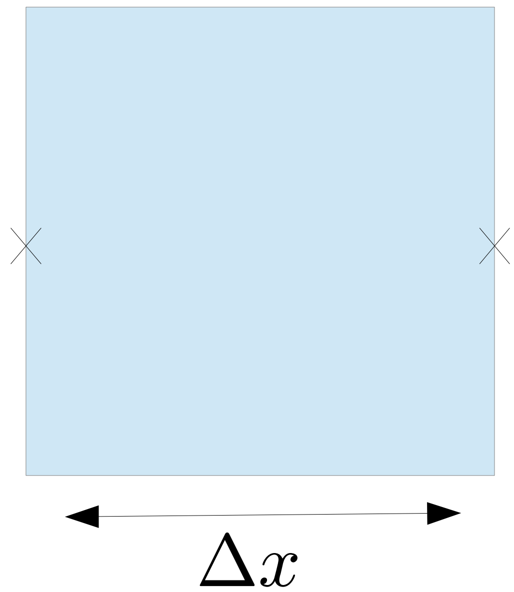
- Limit is a continuous function
- Here a function of two variables

$$f = f(x, y)$$

- As we move in either x or y direction the value of f changes

Two Dimensions and Partial Derivatives

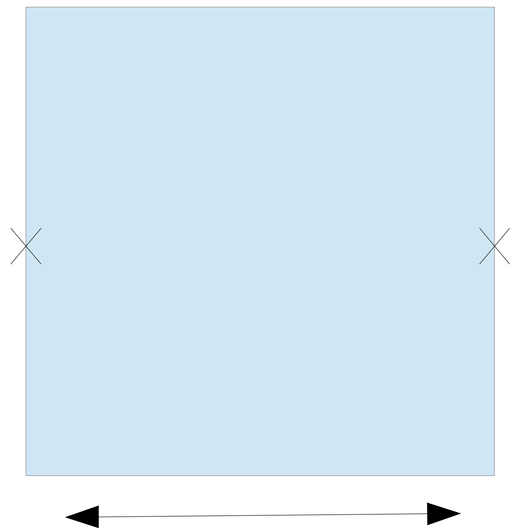
$$f(x, y + \frac{\Delta y}{2})$$



$$f(x + \Delta x, y + \frac{\Delta y}{2})$$

Two Dimensions and Partial Derivatives

$$f(x, y + \frac{\Delta y}{2})$$



$$\Delta x$$

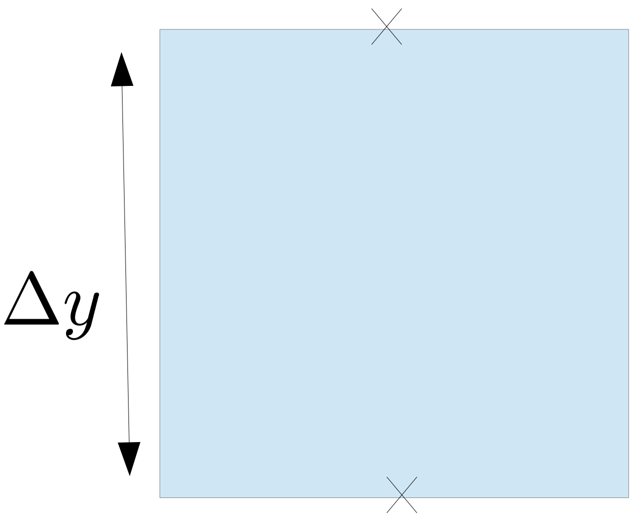
$$f(x + \Delta x, y + \frac{\Delta y}{2})$$

- Note we have dropped the half Delta terms for simplicity

$$\frac{\partial f}{\partial x}\Big|_{y \text{ constant}} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x, y) - f(x, y)}{\Delta x}$$

Two Dimensions and Partial Derivatives

$$f(x + \frac{\Delta x}{2}, y + \Delta y)$$

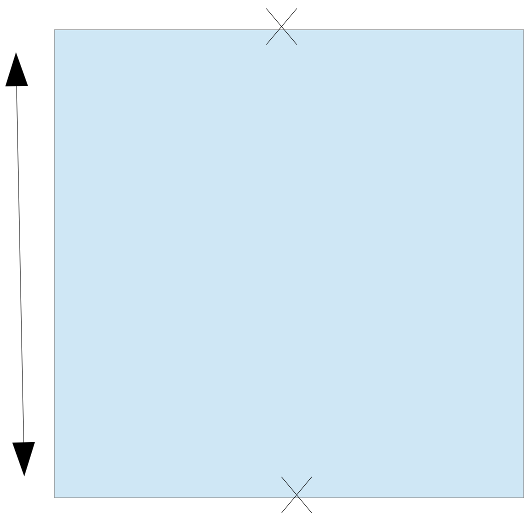


$$f(x + \frac{\Delta x}{2}, y)$$

Two Dimensions and Partial Derivatives

$$f(x + \frac{\Delta x}{2}, y + \Delta y)$$

Δy



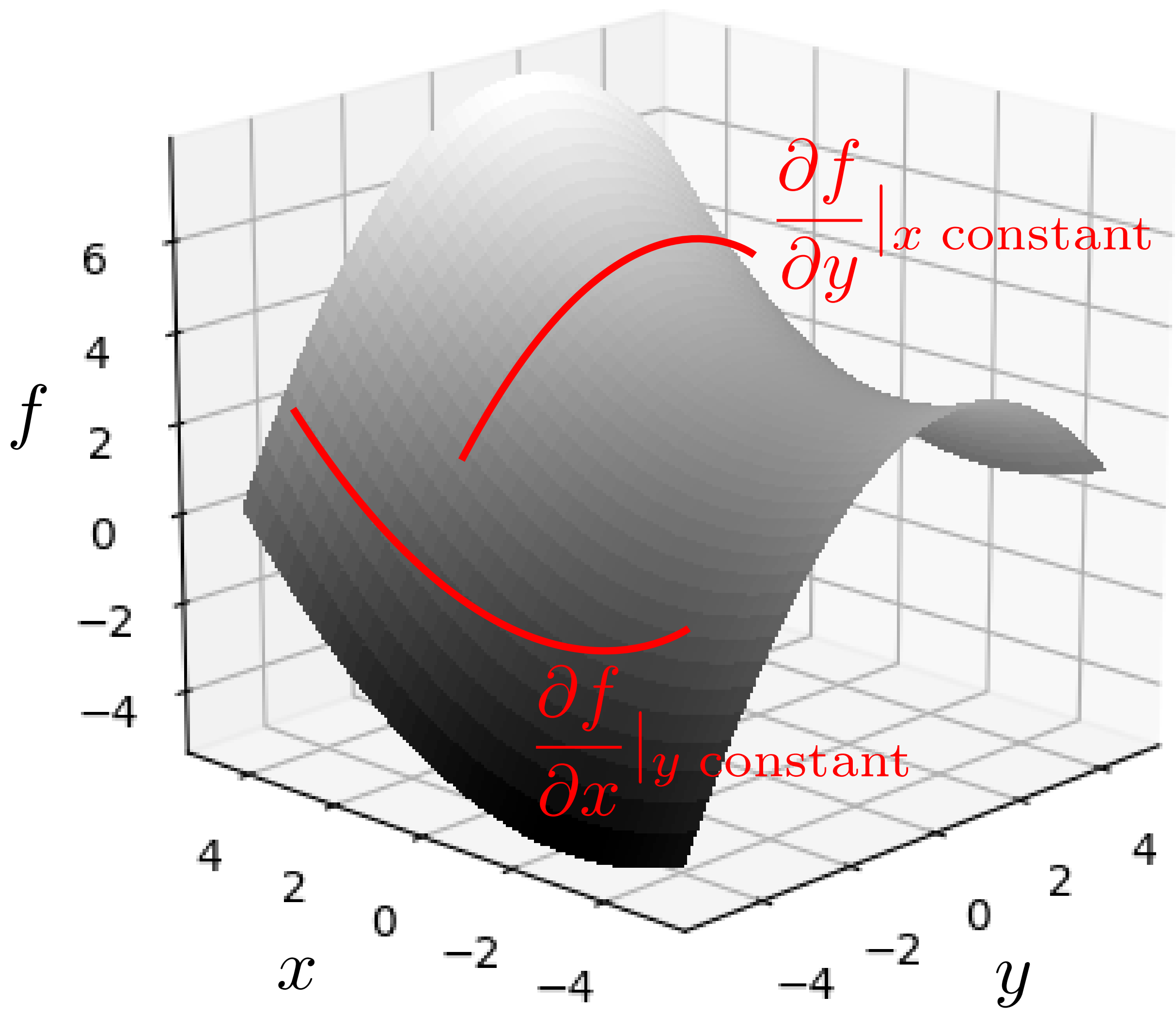
- Note we have dropped the half Delta terms for simplicity

$$\frac{\partial f}{\partial y}\Big|_{x \text{ constant}}$$

$$= \lim_{\Delta y \to 0} \frac{f(x, y + \Delta y) - f(x, y)}{\Delta y}$$

$$f(x + \frac{\Delta x}{2}, y)$$

Two Dimensions and Partial Derivatives



- Consider a function of two variables

$$f = f(x, y)$$

$$\frac{\partial f}{\partial x}\Big|_{y \text{ constant}}$$

$$\frac{\partial f}{\partial y}\Big|_{x \text{ constant}}$$

Example of a Field and it's Derivatives

- Consider an example field described by an x-y polynomial

$$f(x, y) = ax^2 + bx + cy^2 + dy + exy + f$$

- We can calculate the derivatives at any point

$$\frac{\partial f}{\partial x}|_{y \text{ constant}} = 2ax + b + ey$$

$$\frac{\partial f^2}{\partial x^2}|_{y \text{ constant}} = 2a$$

$$\frac{\partial f}{\partial y}|_{x \text{ constant}} = 2cy + d + ex$$

$$\frac{\partial f^2}{\partial y^2}|_{y \text{ constant}} = 2c$$

Example of a Field and it's Derivatives

- Consider an example field described by an x-y polynomial

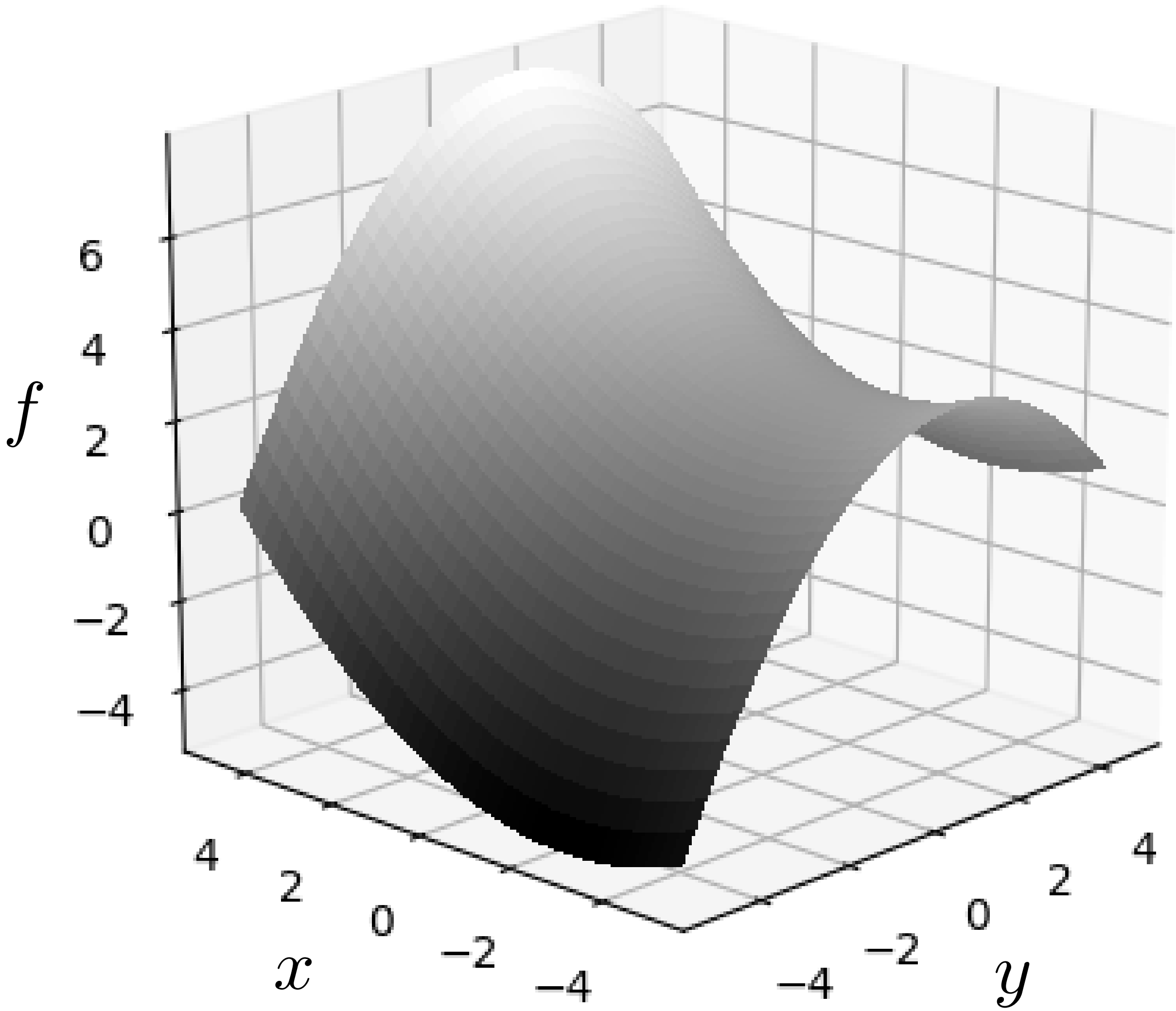
$$f(x,y) = ax^2 + bx + cy^2 + dy + exy + f$$

- We can also calculate the derivatives numerically (note the subscript notation is used again but in 2D with i and j)

$$\frac{\partial f}{\partial x} \approx \frac{f(x+\Delta x, y) - f(x,y)}{\Delta x} \equiv \frac{f_{i+1,j} - f_{i,j}}{\Delta x}$$

$$\frac{\partial f}{\partial y} \approx \frac{f(x, y+\Delta y) - f(x,y)}{\Delta y} \equiv \frac{f_{i,j+1} - f_{i,j}}{\Delta y}$$

Plotting Fields (3D plot)



- Limit is a continuous function
- Here a function of two variables

$$f = f(x, y)$$

- As we move in either x or y direction the value of f changes

Plotting Fields (3D plot Code)

```
from mpl_toolkits.mplot3d import Axes3D
from matplotlib.pyplot import *
from numpy import *

#Constants
a = -0.2; b = 0.5; c=0.1; d=0.5; e=0.; f=3.
Npoints = 50

#Define Domain
X = linspace(-5, 5, Npoints)
Y = linspace(-5, 5, Npoints)
X, Y = meshgrid(X, Y)
Z = a*X**2 + b*X + c*Y**2. + d*Y + e*X*Y + f

#Plot 3D figure
fig = figure()
ax = fig.gca(projection='3d')
surf = ax.plot_surface(X, Y, Z, cmap=cm.gray)
fig.colorbar(surf)
show()
```

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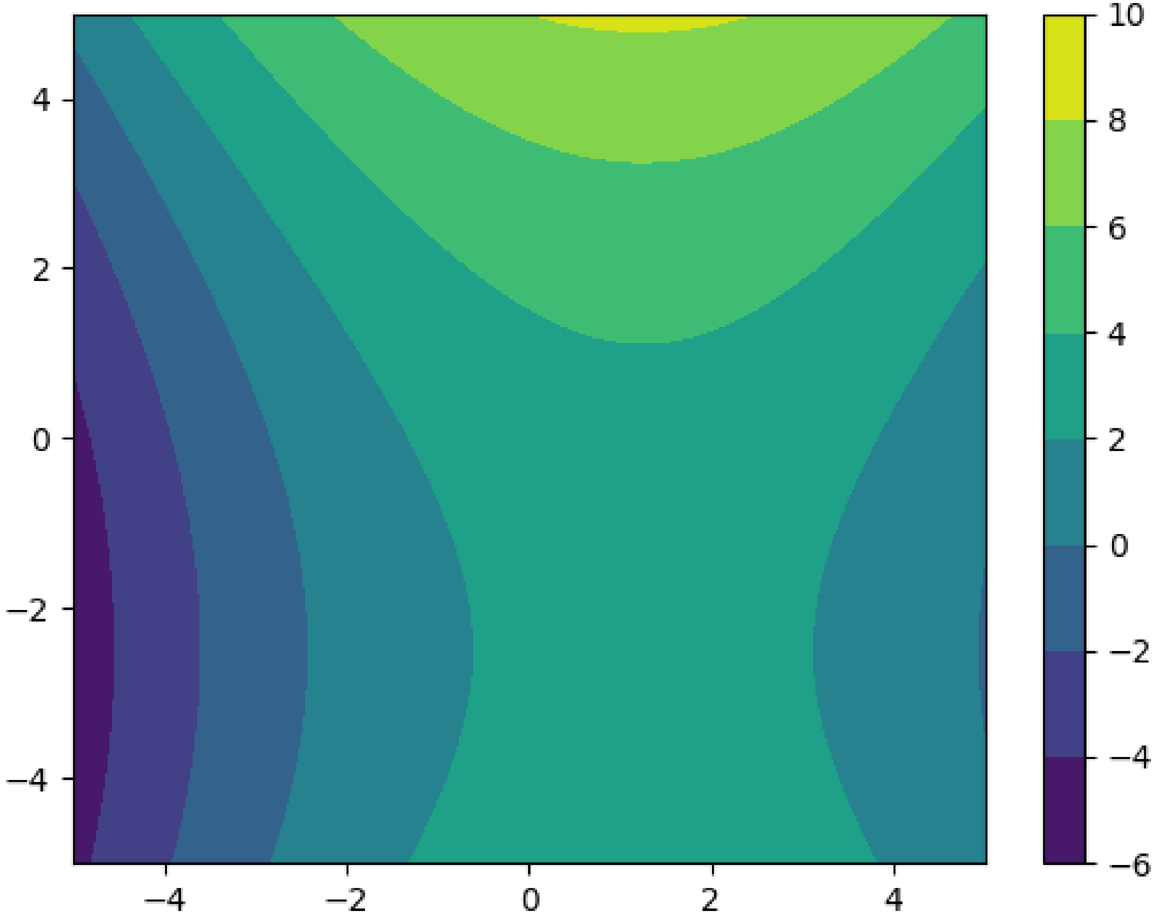
Plotting Fields (2D plot)

- Contour plot



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Plotting Fields (2D plot Code)

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from numpy import *

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X = linspace(-5, 5, Npoints)
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X, Y = meshgrid(X, Y)
Z = a*X**2 + b*X + c*Y**2. + d*Y + e*X*Y + f

#Plot 2D figure
contourf(X, Y, Z)
colorbar()
show()
```

Questions 2

- Plot the following field as a contour (Python/MATLAB/excel)

$$f(x, y) = \sin(2\pi x)\cos(2\pi y) \text{ for } 0 < x < 1 \text{ and } 0 < y < 1$$

- Evaluate partial derivatives in x and y and plot these fields

$$\frac{\partial f}{\partial x}\Big|_{y \text{ constant}} \qquad \frac{\partial f}{\partial y}\Big|_{x \text{ constant}}$$

- Calculate the numerical derivatives of f(x,y) and compare to the partial derivatives from part 2. What happens if you increase the number of points you use?

$$\frac{\partial f}{\partial x} \approx \frac{f_{i+1,j} - f_{i,j}}{\Delta x} \qquad \frac{\partial f}{\partial y} \approx \frac{f_{i,j+1} - f_{i,j}}{\Delta y}$$

Solving Partial Differential Equations

Partial Differential Equations

- To describe the change in fields, we use partial differential equations which vary in space (2D here), for example:

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

- Note we have dropped the x=constant, y=constant for notational conciseness, but they are <u>always</u> implied by partial derivatives

- This equation describes the final state for the process of diffusion of a substance, such as ink in water or concentration of a chemical in a mixture. It can also be solved to define electromagnetic fields or potential fluid flow

Partial Differential Equations

- This equation is known as Laplace's Equation

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

- Often written using other notation,

$$\nabla^2 f = 0 \text{ or } \Delta f = 0 \text{ where } \nabla^2 \equiv \Delta \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$$

$$f_{xx} + f_{yy} = 0 \text{ where subscripts denote derivatives}$$

- In practice, fields are usually a function of three spatial coordinates and time (2D here for simplicity)

$$f = f(x, y, z, t)$$

Solving Numerically

- There are a number of analytical solutions to this equation

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

- But we will use numerical solutions, recall the numerical approximation for the second derivative, adapted for 2D,

$$\frac{\partial^2 f}{\partial x^2} \approx \frac{f(x + \Delta x, y) - 2f(x, y) + f(x - \Delta x, y)}{(\Delta x)^2}$$

$$\frac{\partial^2 f}{\partial y^2} \approx \frac{f(x, y + \Delta y) - 2f(x, y) + f(x, y - \Delta y)}{(\Delta y)^2}$$

Solving Numerically

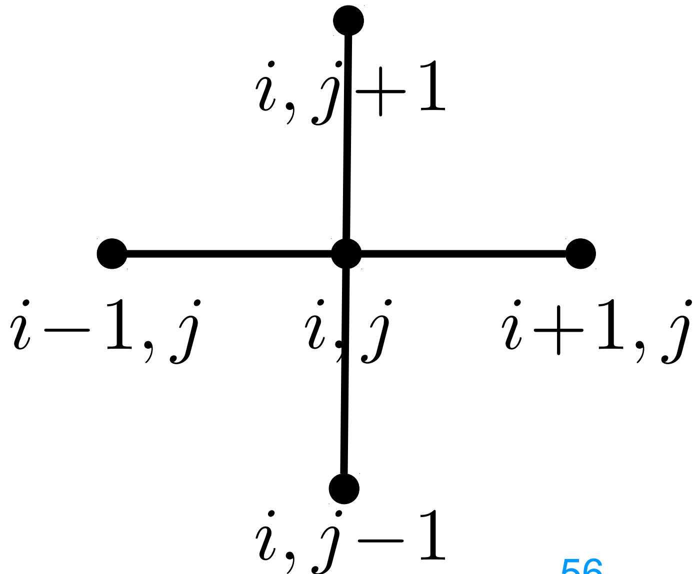
- There are a number of analytical solutions to this equation

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

- But we will use numerical solutions, written here in index notation which shows the "stencil"

$$\frac{\partial^2 f}{\partial x^2} \approx \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{(\Delta x)^2}$$

$$\frac{\partial^2 f}{\partial y^2} \approx \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{(\Delta y)^2}$$



Solving Numerically

- So we are solving $$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0$$

$$\frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{(\Delta x)^2} + \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{(\Delta y)^2} = 0$$

- Which we rearrange to give

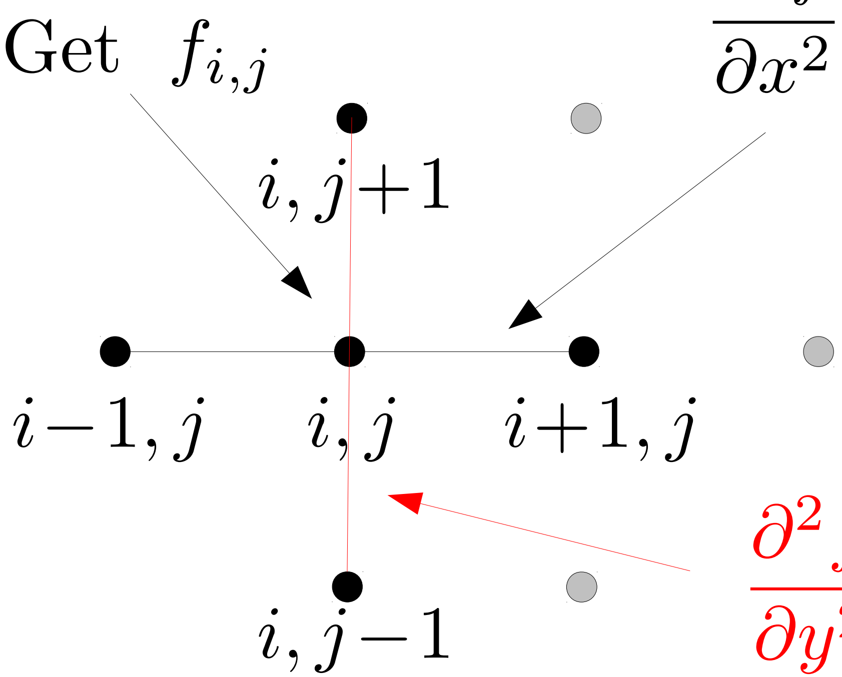
$$f_{i,j} = \frac{1}{2}\frac{(\Delta x)^2(\Delta y)^2}{(\Delta x)^2 + (\Delta y)^2}\left[\frac{f_{i+1,j} + f_{i-1,j}}{(\Delta x)^2} + \frac{f_{i,j+1} + f_{i,j-1}}{(\Delta y)^2}\right]$$

$$f_{i,j} = \frac{1}{4}\left[\frac{f_{i+1,j} + f_{i-1,j}}{(\Delta x)^2} + \frac{f_{i,j+1} + f_{i,j-1}}{(\Delta y)^2}\right] \quad \Delta x = \Delta y = 1$$

Boundary Conditions

- Notice that if we solve this equation, we use points either side

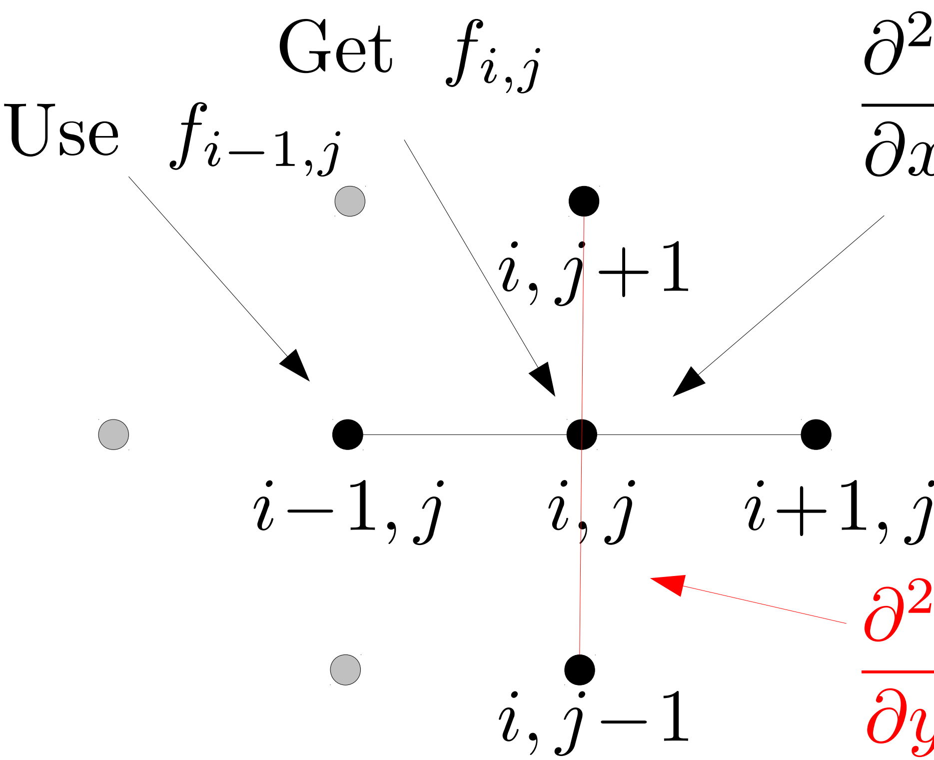
$$\frac{\partial^2 f}{\partial x^2} \approx \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{(\Delta x)^2}$$



$$\frac{\partial^2 f}{\partial y^2} \approx \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{(\Delta y)^2}$$

Boundary Conditions

- Notice that if we solve this equation, we use points either side
- Then we move to the next point

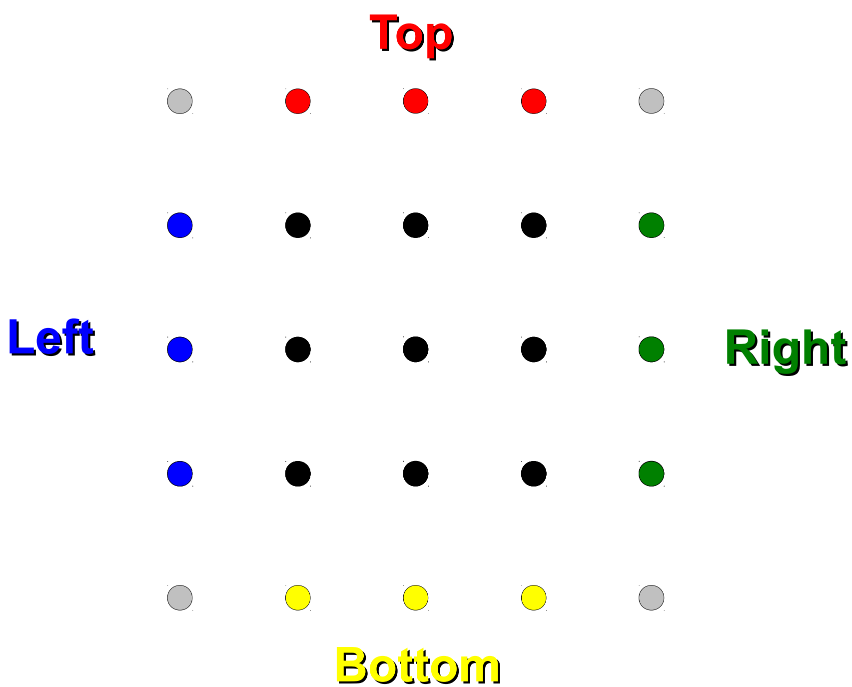


$$\frac{\partial^2 f}{\partial x^2} \approx \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{(\Delta x)^2}$$

$$\frac{\partial^2 f}{\partial y^2} \approx \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{(\Delta y)^2}$$

Boundary Conditions

- Notice that if we solve this equation, we use points either side
- Then we move to the next point
- We start from the edge of our domain (boundary)
- These boundary values must be specified and determine the solution we get from solving Laplace's equation



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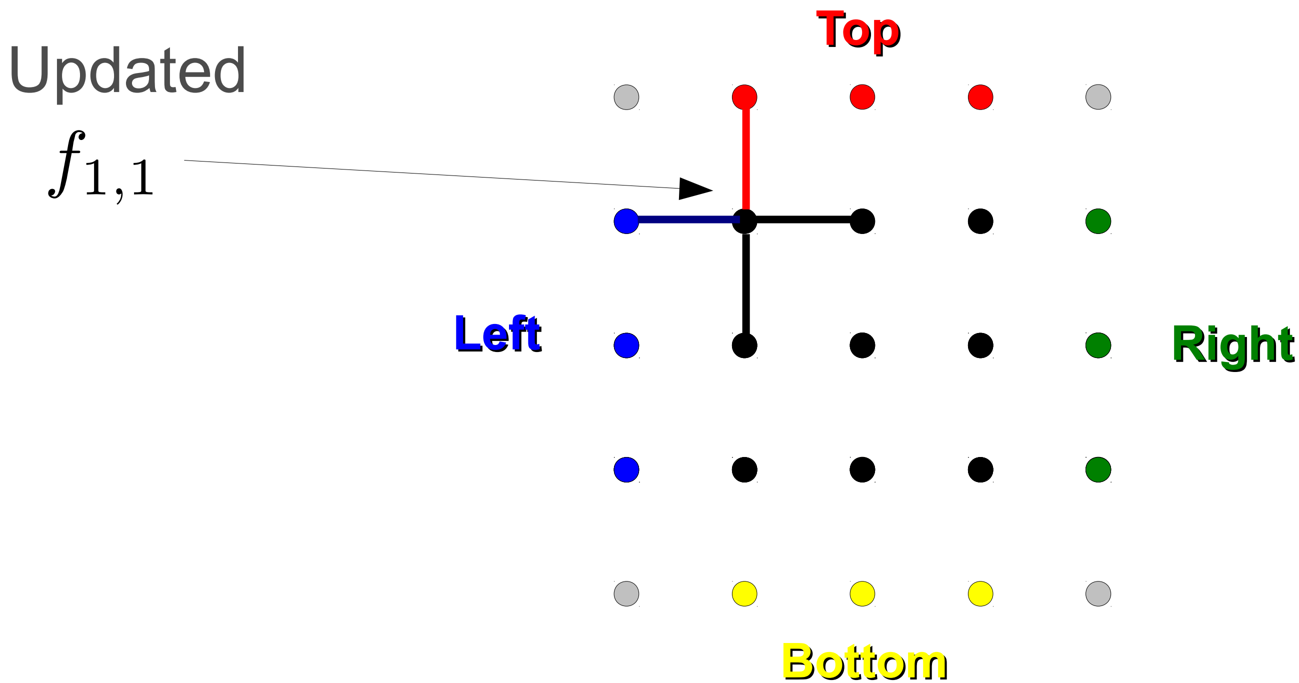

Boundary Conditions

- Notice that if we solve this equation, we use points either side
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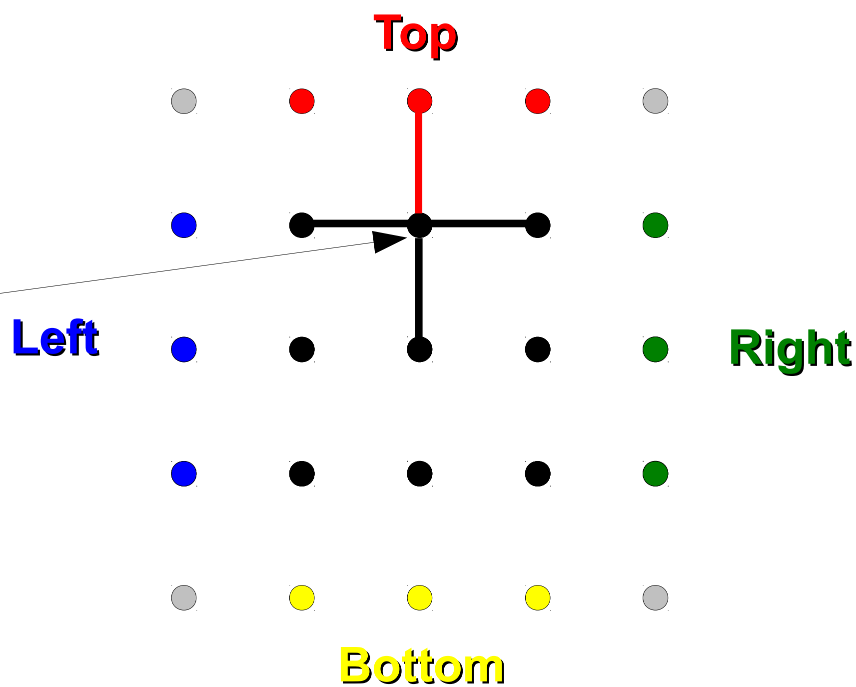
- We start from the edge of our domain (boundary)
- These boundary values must be specified and determine the solution we get from solving Laplace's equation

Updated $f_{1,1}$

Updated $f_{2,1}$



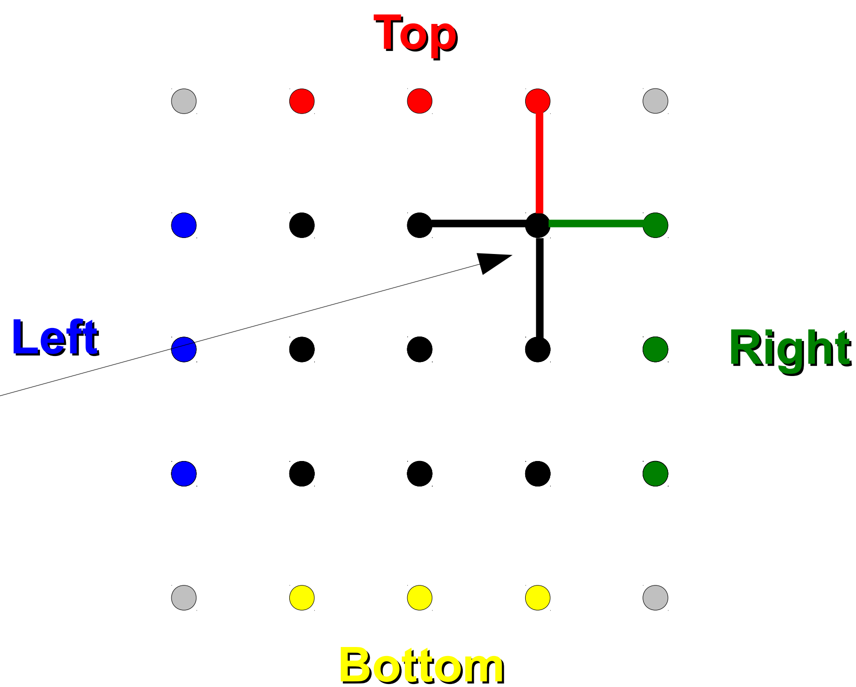
Boundary Conditions

- Notice that if we solve this equation, we use points either side
- Then we move to the next point
- We start from the edge of our domain (boundary)
- These boundary values must be specified and determine the solution we get from solving Laplace's equation

Updated $f_{1,1}$

Updated $f_{2,1}$

Updated $f_{3,1}$



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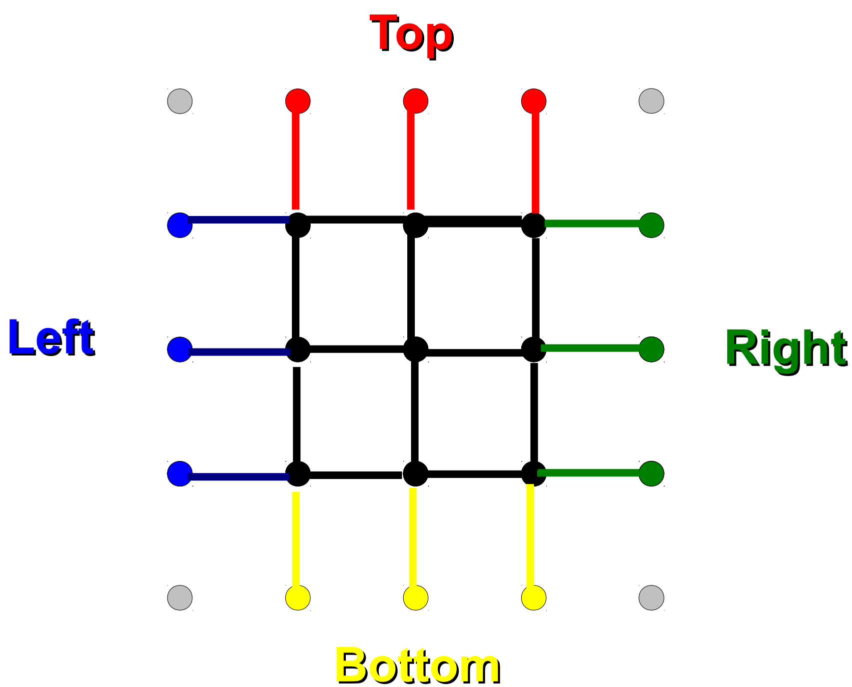
Boundary Conditions

- Proceed until all 9 internal values (in black) are updated

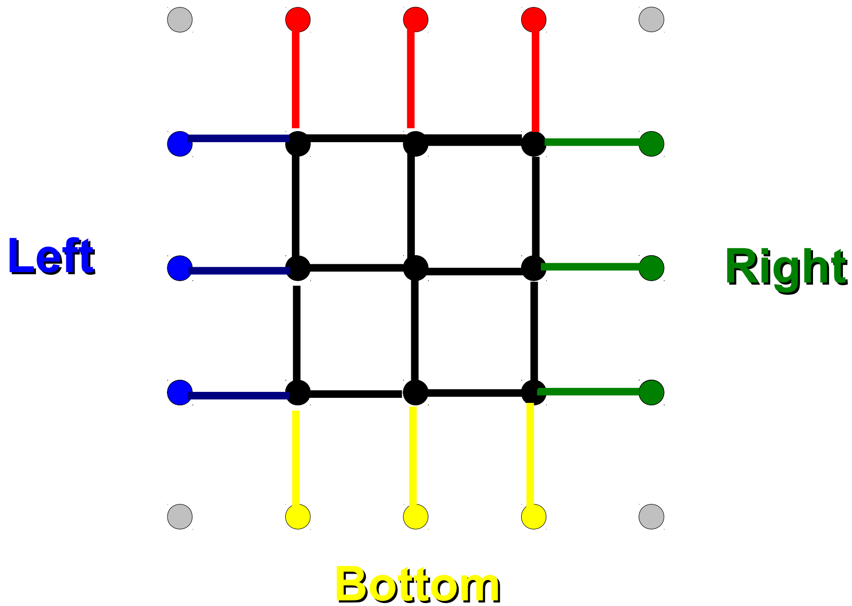
Updated $f_{1,1}$ $f_{2,1}$ $f_{3,1}$ $f_{1,2}$ $f_{2,2}$ $f_{3,2}$ $f_{1,3}$ $f_{2,3}$ $f_{3,3}$

- We then repeat the process again starting from these updated values



Boundary Conditions

- Iteration should proceeds until a solution is reached, convergence check: $$\left| \sum_{i=1}^{9}\sum_{j=1}^{9} f_{i,j} - \sum_{i=1}^{9}\sum_{j=1}^{9} f_{i,j}^{\text{Previous Iteration}} \right| < \epsilon$$
- Iteration must be turned on in Excel (options) or explicitly iterated using a loop in Python/MATLAB



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Questions 3

- Starting from Laplace's equation: derive the approximation for fij,

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

$$f_{i,j} = C\left[\frac{f_{i+1,j} + f_{i-1,j}}{(\Delta x)^2} + \frac{f_{i,j+1} + f_{i,j-1}}{(\Delta y)^2}\right]$$

- Where $C = 1/4$
- Solve with Python, MATLAB or Excel for 9 points, N.B. this must be iterated. Try the following boundary conditions:
  - Top =0, Bottom =1, Left=1, Right=0
  - Top = 1, Bottom=0 and use Periodic Boundaries for others, i.e. for Left = Copy right cell-1 and for Right=Copy left cell+1
  - Top = 0, Bottom=0, Left = sin(pi y), Right = 0 with 0<y<1
  - Before next week: Make sure you understand this. Comment your code, try different numbers of points in the domain, try plotting, test other boundaries. Make notes on what you observe.

Summary

- In today's session you have:
  - Seen what the Continuum assumption means and been shown that, crucially, it describes continuous fields
  - An introduction to fields and how to plot them
  - Been introduced to some simple ordinary and partial differential equations
  - Been shown how to solve basic differential equations numerically
  - Tried to solve them using either a programming language of your choice or Excel

Scalar, Vector and Tensor Fields

- Note that the fields can also be scalar, vector or even tensor fields. Examples include:
  - Pressure, Concentration of chemical species

$$P = P(x, y, z, t) \qquad C = C(x, y, z, t)$$

  - Velocity (3 values at every space and time)

$$\underline{u} = \underline{u}(x, y, z, t) = \begin{pmatrix} u \\ v \\ w \end{pmatrix}$$

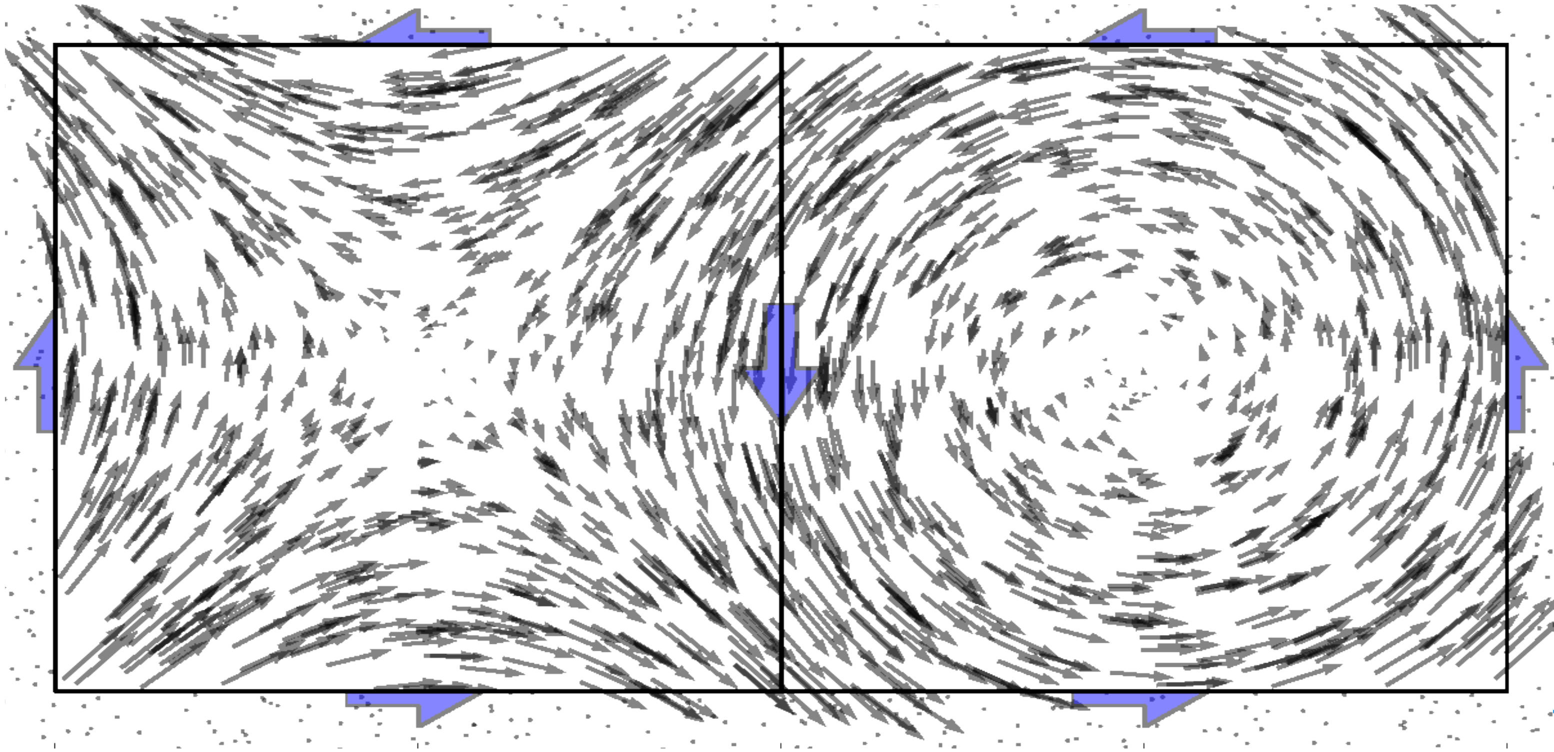
  - Stress tensor (9+ values)

$$\underline{\underline{\Pi}} = \underline{\underline{\Pi}}(x, y, z, t) = \begin{pmatrix} \Pi_{xx} & \Pi_{xy} & \Pi_{xz} \\ \Pi_{yx} & \Pi_{yy} & \Pi_{yz} \\ \Pi_{zx} & \Pi_{zy} & \Pi_{zz} \end{pmatrix}$$

Scalar, Vector and Tensor Fields

- 2D Velocity Fields example (2 values at every space)

$$\underline{u} = \underline{u}(x, y) = \begin{pmatrix} u \\ v \end{pmatrix}$$



The Navier-Stokes Equation

- Describes the flow of single phase Newtonian fluids

$$\underbrace{\frac{\partial \underline{u}}{\partial t}}_{\text{Unsteady Term}} + \underbrace{\underline{u} \cdot \underline{\nabla}\, \underline{u}}_{\text{Convection Term}} = -\underbrace{\frac{1}{\rho} \underline{\nabla} P}_{\text{Pressure Term}} + \nu \underbrace{\nabla^2 \underline{u}}_{\text{Laplace's Equation}}$$

- Lots of complexity here – we'll cover in next few lessons
- Velocity vector equation so actually three simultaneous equations connected by scalar pressure P

Plan for the Continuum Part of the Course

- Where we are in the wider modelling hierarchy
- Understand the Continuum assumption
- Partial differential equations and numerical solutions

Session 1

- More partial differential equations and numerical solutions
- Two dimensional vector fields
- The Navier-Stokes Equation
  - Assumptions that lead to it
  - Key terms and their meaning (with some extensions)
  - Simplifications and solutions

Session 2

- Link to the molecular dynamics equations
- Numerical solutions to the Navier-Stokes equation

Session 3

Further Reading

- Differential Equations
  - Engineering Mathematics by K. A. Stroud
- Fluid Dynamics and CFD
  - Hirsch (2007) ”Numerical Computation of Internal and External Flows” Elsevier
  - 12 Step Navier Stokes (http://lorenabarba.com/blog/cfd-python-12-steps-to-navier-stokes/)
- Introduction to links to other scales (next week)
  - Mohamed Gad-El-Hak (2006) Gas and Liquid Transport at the Microscale, Heat Transfer Eng., 27:4, 13-29,
  - Irving and Kirkwood (1950) The Statistical Mechanics Theory of Transport Process IV, J. Chem Phys