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The Continuum

Multi-Scale Modelling IMSE

Part 2
15th 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

- Link to the molecular dynamics equations
- The Navier-Stokes Equation
  - Assumptions that lead to it
  - Key terms and their meaning (with some extensions)
  - Simplifications and solutions
- More partial differential equations and numerical solutions

Session 2

- Assessed exercise - numerical solutions to the Navier-Stokes equation

Session 3

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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:
  - Been reminded of vector and tensor fields with a review of vector notation
  - Seen the derivation of the Navier-Stokes equation
  - Understand the link to discrete systems and the impact of the choice of reference frame
  - Have an idea of the assumptions made to get the continuum fluid dynamics equations of motion
  - Seen the physical interpretation of the various terms and how to simplify the equation
  - A review of solving differential equations numerically applied to a simplified Navier-Stokes equation

Review

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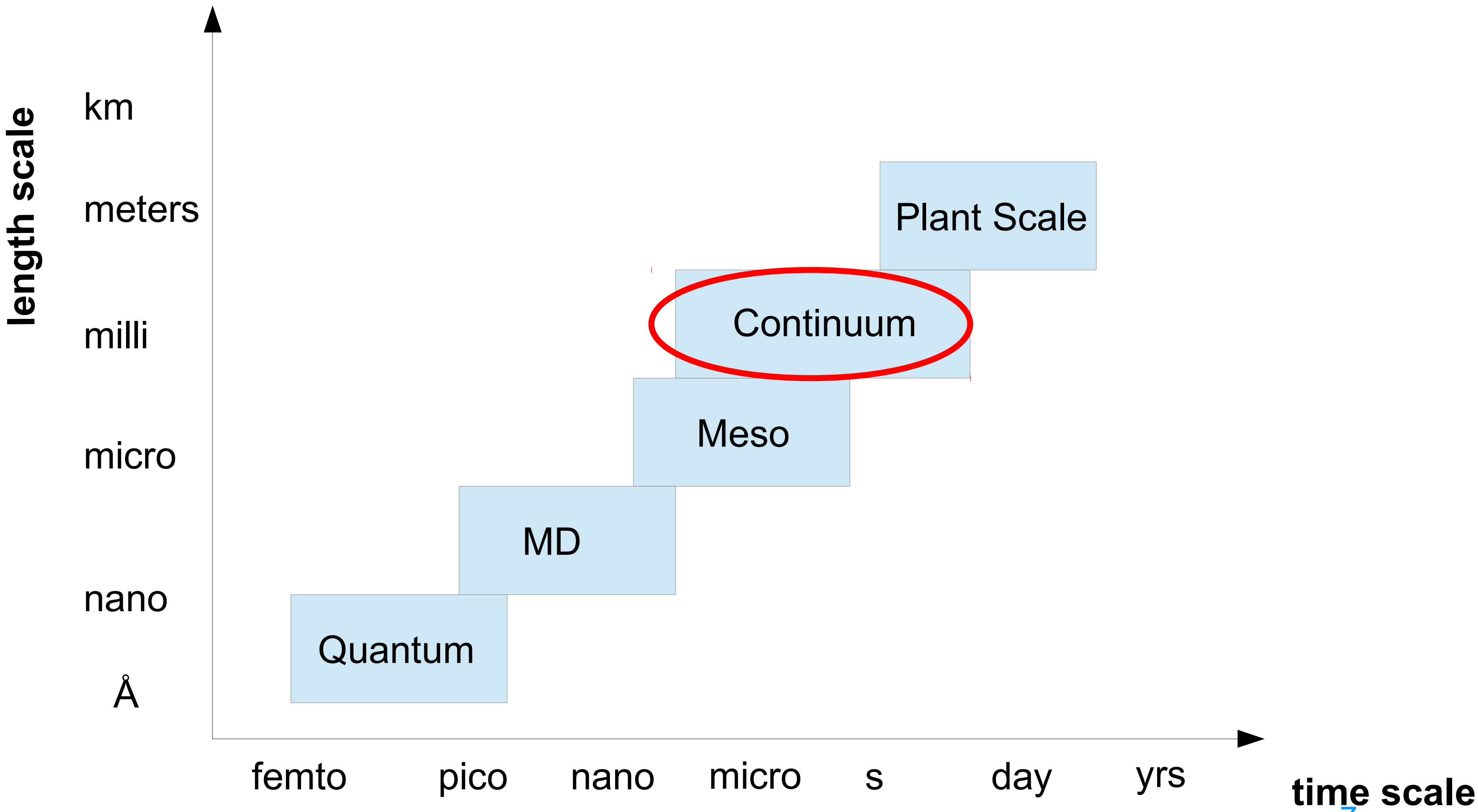
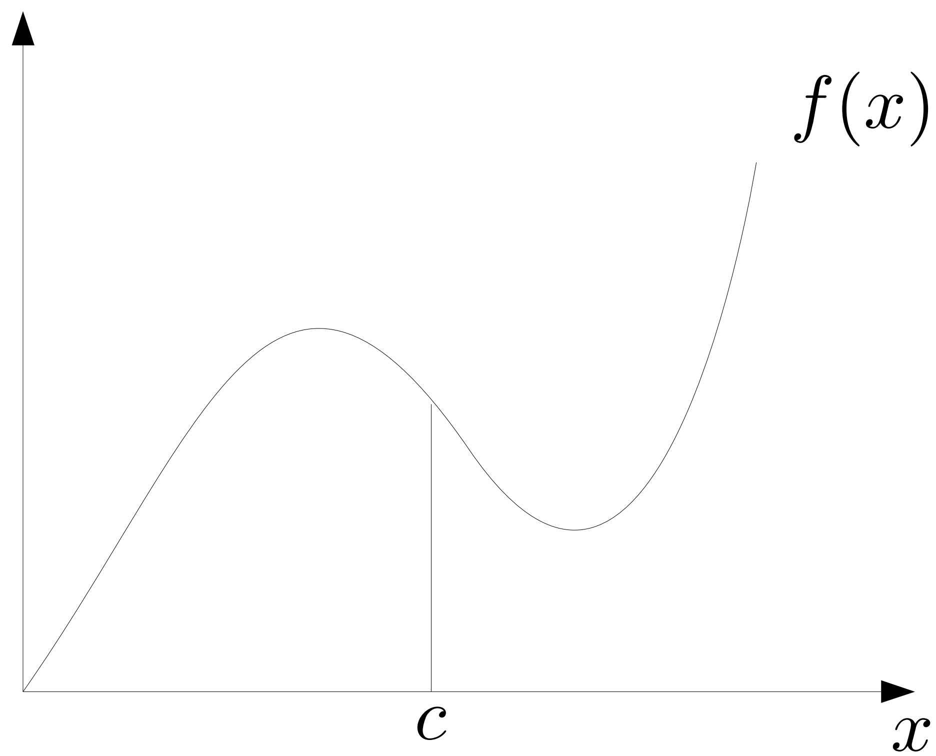
Scale Hierarchy



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.

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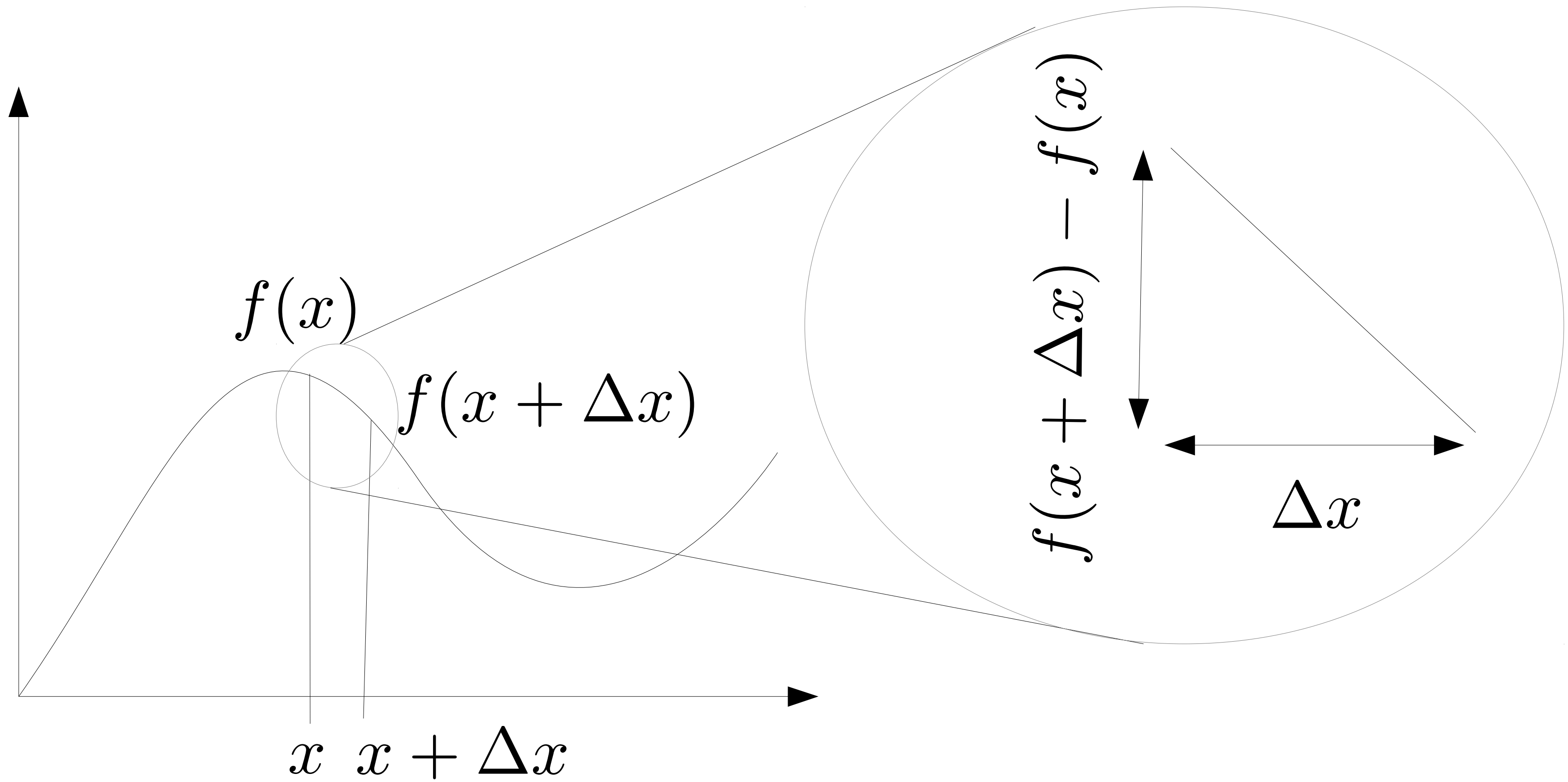
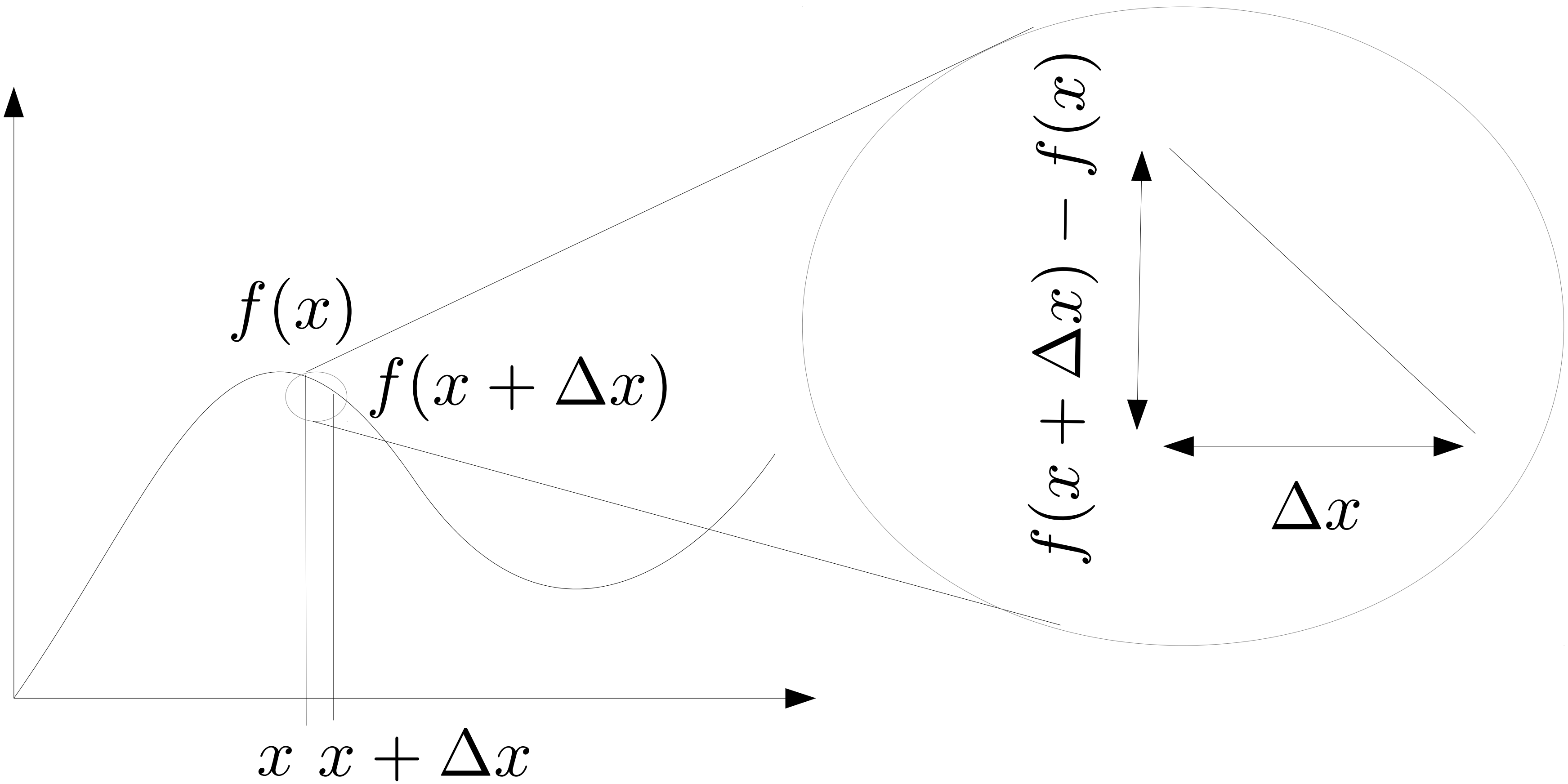
Definition of a Derivative



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

Definition of a Derivative



Better with smaller Δx

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

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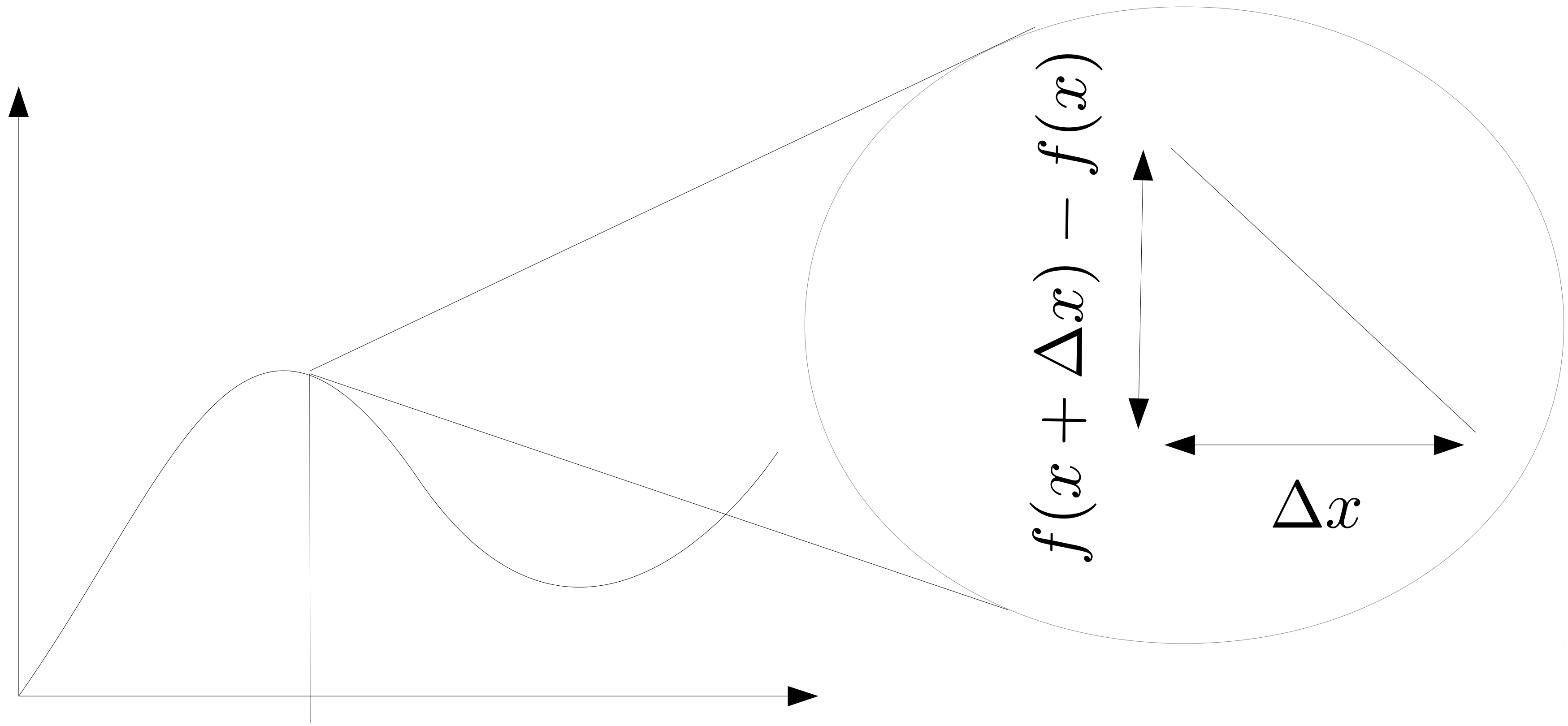
Definition of a Derivative



Exact in Limit $\Delta x \to 0$

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

Continuum Fields

- MD uses Newton's law assuming continuity in time and position in a discrete molecular system
- The Continuum hypothesis therefore refers to the continuous fields in space. These are 2D or 3D continuous functions evolving 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
- The largest molecular simulations are of order 10^{9} which is still only micro-meters. System size is prohibitive

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The Navier-Stokes Equation

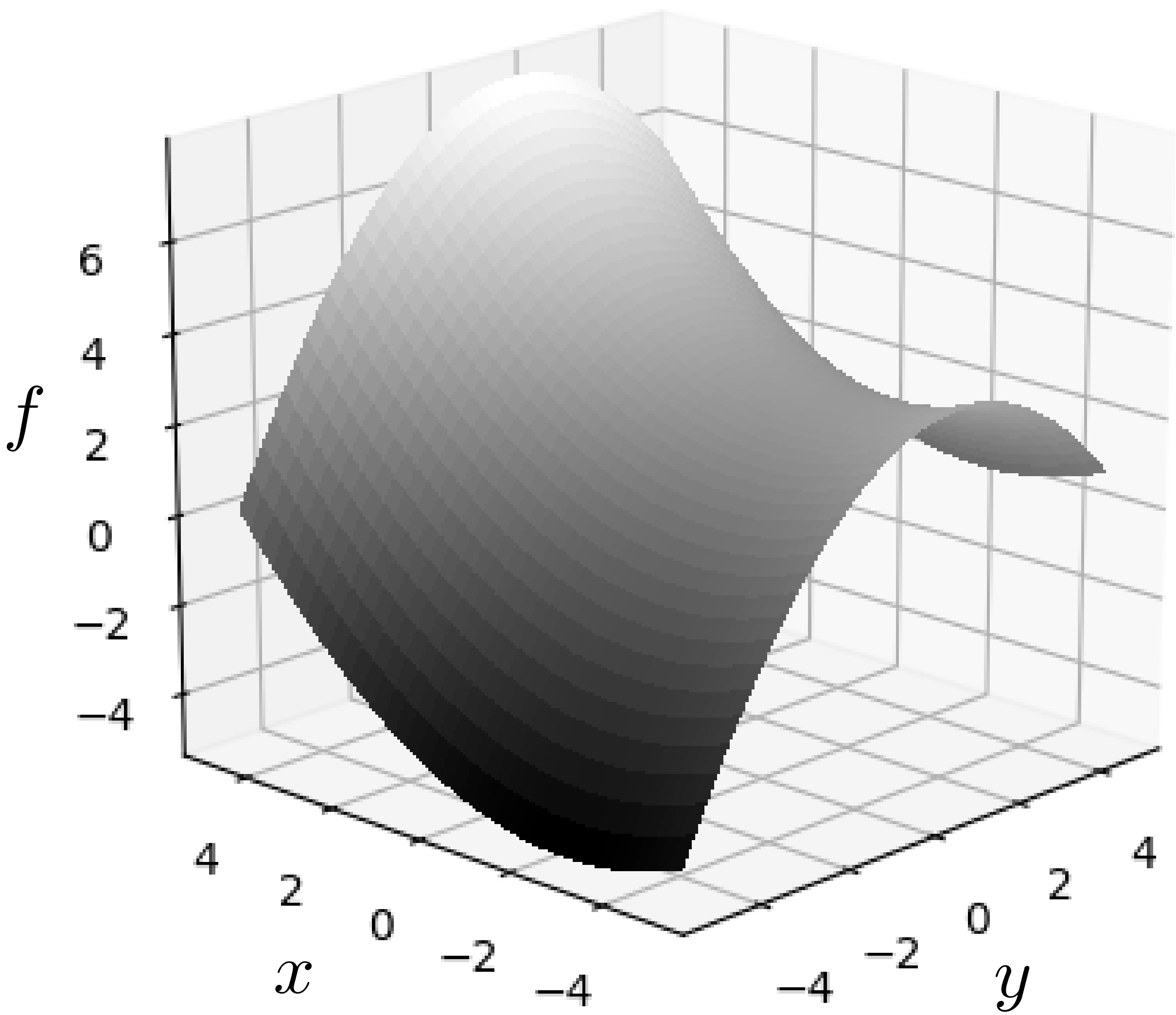
- Describes the flow of single phase Newtonian fluids

last week

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

- Lots of complexity here
- Velocity vector equation so actually three simultaneous equations connected by scalar pressure P

Two Dimensions and Partial Derivatives



- A 2D field is a function of two variables

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

- Show here in 3D for visualisation
- Assumed to be a continuous function

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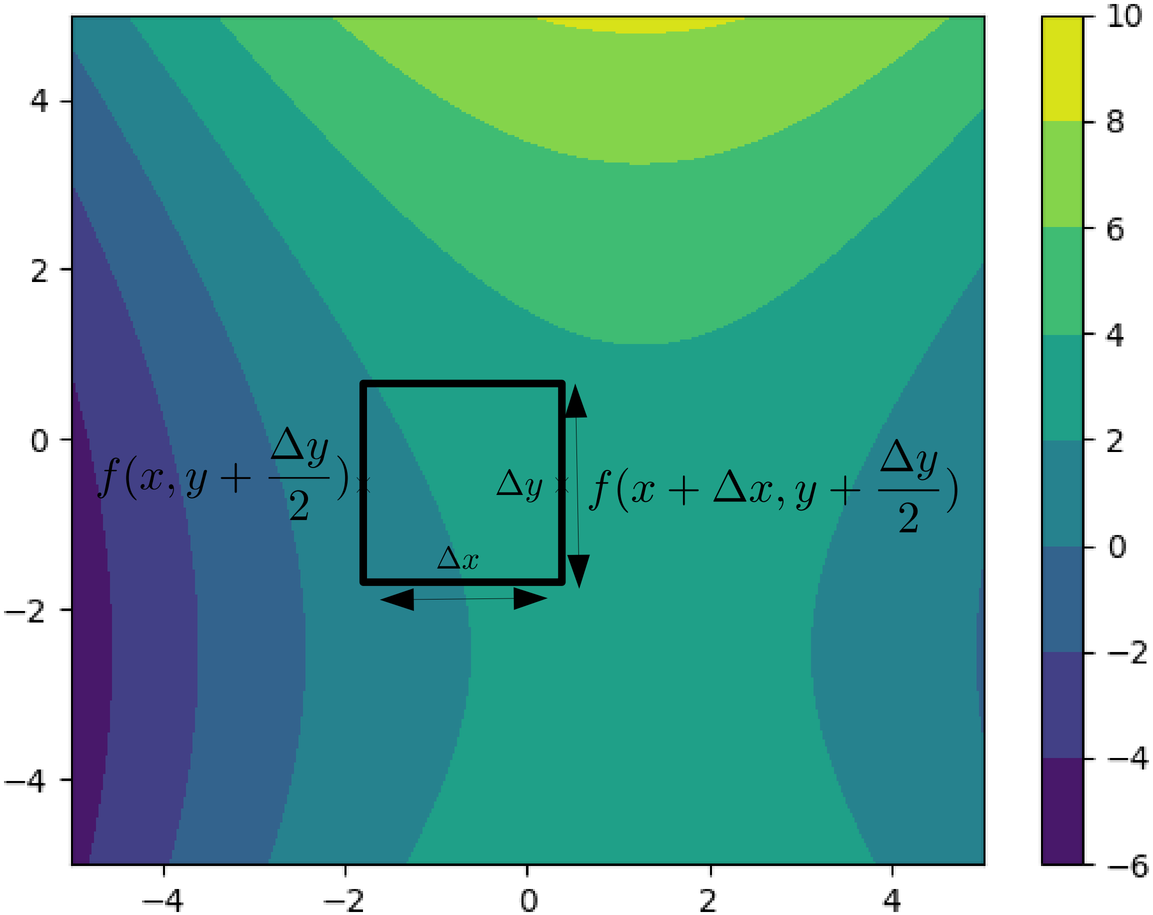
Get MATLAB Plots Working

```
x = linspace(-5, 5., 100);
y = linspace(-5, 5., 100);
[X, Y] = meshgrid(x, y);

a = -0.2; b = 0.5; c=0.1;
d=0.5; e=0.; f=3.

u = a*X.^2 + b*X + c*Y.^2 + d*Y + e*X.*Y + f;

contourf(X, Y, u)
%surf(X, Y, u)
colorbar
```

Two Dimensions Fields (2D plot)

- Contour plot



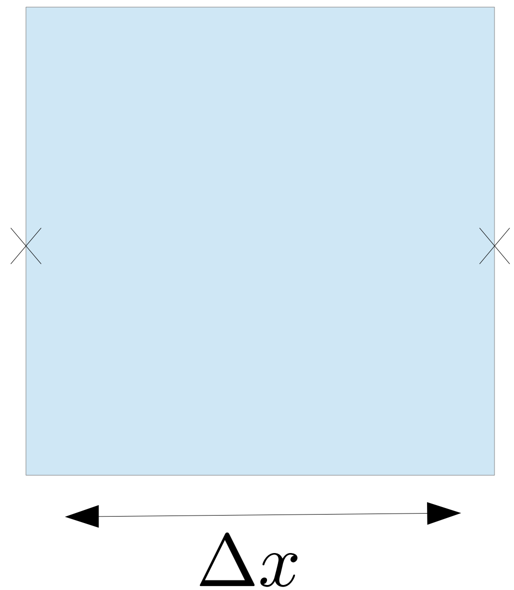
- Limit is a continuous function
- Here a function of two variables

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

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

Two Dimensions and Partial Derivatives

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



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

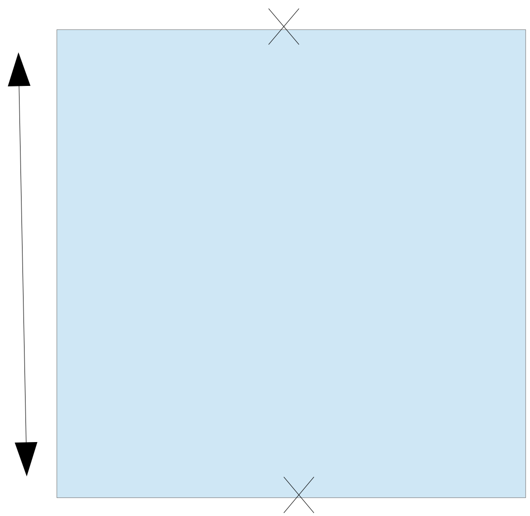
- Note we have dropped the half Delta terms for simplicity

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

Two Dimensions and Partial Derivatives

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

$$\Delta y$$



- Note we have dropped the half Delta terms for simplicity

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

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

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

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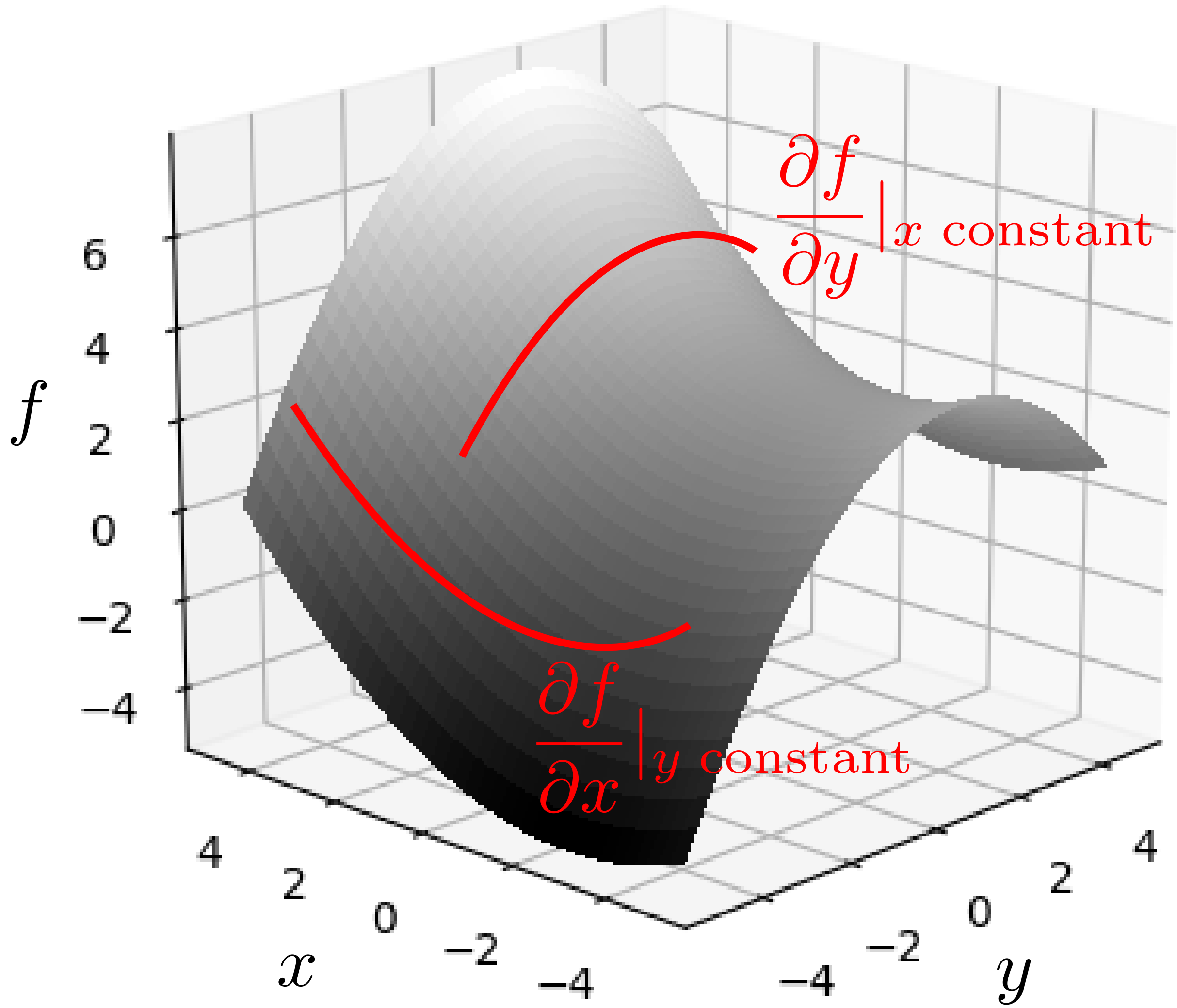
Two Dimensions and Partial Derivatives



- Consider a function of two variables

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

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

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

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Vector Fields

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)

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

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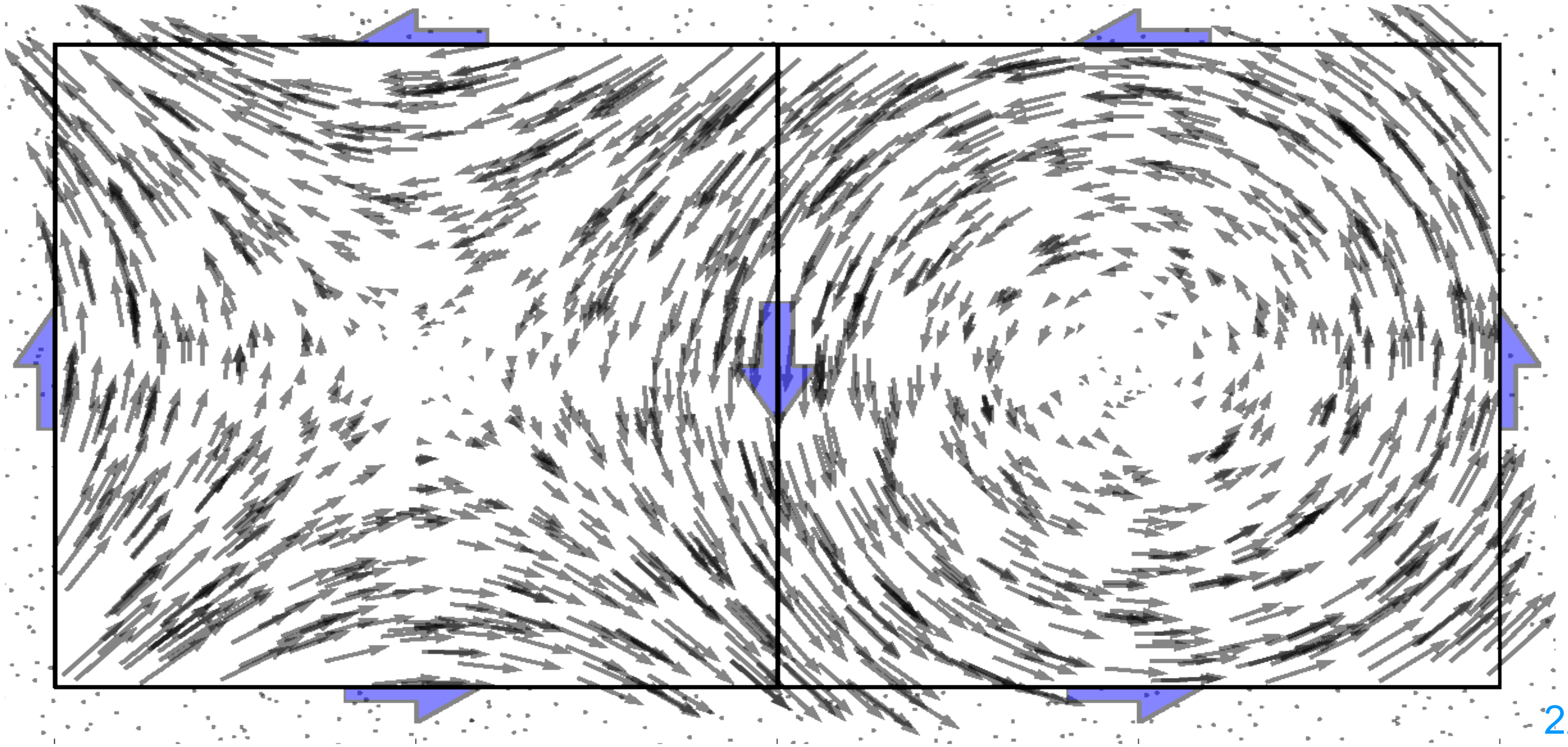
Scalar, Vector and Tensor Fields

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

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



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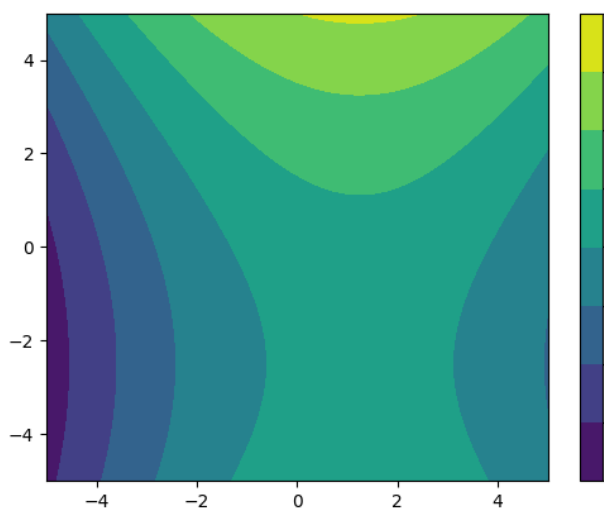
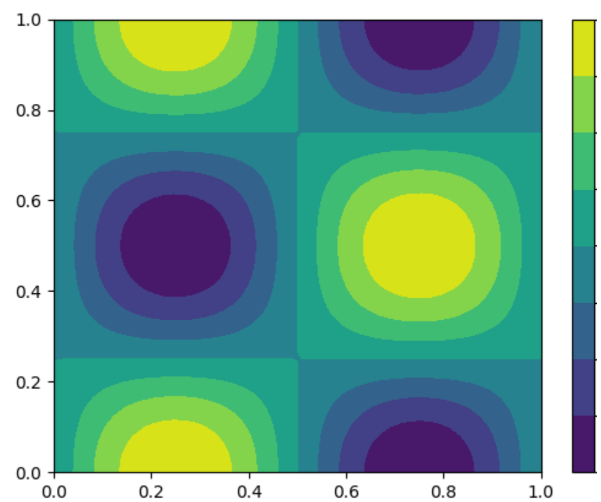
Example of a Vector Field

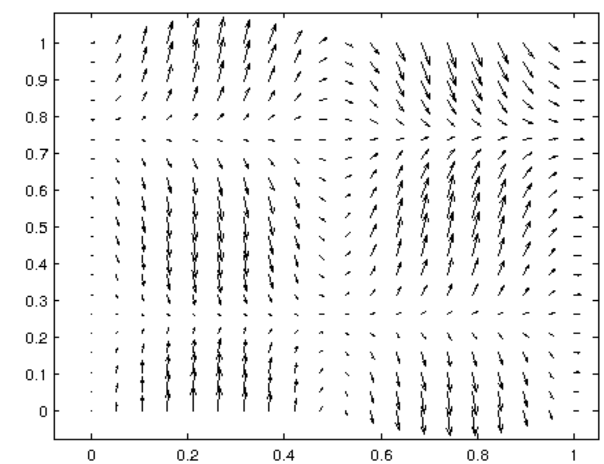
- We combine our two examples from last week The example 2D field described by an x-y polynomial in u and sine and cosine function in v

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

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







MATLAB quiver Plots

```
x = linspace(0, 1., 20);
y = linspace(0, 1., 20);
[X, Y] = meshgrid(x, y);

a = 0.01; b = 0.02; c = 0.01;
d = 0.01; e = 0.1; f = 0;

u = a*X.^2 + b*X + c*Y.^2 + d*Y + e*X.*Y + f;
v = sin(2*pi*X).*cos(2*pi*Y);

quiver(X, Y, u, v, 1., 'k')
```

Vector Calculus

- The upside-down triangle (Nabla) in the Navier-Stokes equation is a vector operator defined as follows,

$$\underline{\nabla} = \underline{i}\frac{\partial}{\partial x} + \underline{j}\frac{\partial}{\partial y} + \underline{k}\frac{\partial}{\partial z}$$

- So dotting this with a vector (divergence) would give a scalar,

$$\underline{\nabla} \cdot \underline{u} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}$$

- While applying to a scalar gives a vector (gradient)

$$\underline{\nabla} C = \underline{i}\frac{\partial C}{\partial x} + \underline{j}\frac{\partial C}{\partial y} + \underline{k}\frac{\partial C}{\partial z}$$

Vector Calculus

- The upside-down triangle (Nabla) in the Navier-Stokes equation is a vector operator defined as follows,

$$\underline{\nabla} = \underline{i}\frac{\partial}{\partial x} + \underline{j}\frac{\partial}{\partial y} + \underline{k}\frac{\partial}{\partial z}$$

- There is also the dyadic or tensor product

$$\underline{\nabla}\, \underline{u} = \underline{\nabla} \otimes \underline{u} = \begin{pmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{pmatrix}$$

Other notation

Index notation

- A useful notation is to express dimensionality as indices

$$\underline{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix} = u_i = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}$$

$$\underline{\underline{\Pi}} = \Pi_{ij} = \begin{pmatrix} \Pi_{11} & \Pi_{12} & \Pi_{13} \\ \Pi_{21} & \Pi_{22} & \Pi_{23} \\ \Pi_{31} & \Pi_{32} & \Pi_{33} \end{pmatrix}$$

- We can then express vector operations concisely

$$\underline{\nabla} P = \frac{\partial P}{\partial x_i} = \begin{pmatrix} \partial P / \partial x_1 \\ \partial P / \partial x_2 \\ \partial P / \partial x_3 \end{pmatrix}$$

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Index notation

- Three rules of index notation
  1) Each unique index is a dimension, the number of unique indices on each side of the equation must agree

  2) Summation convention (Einstein) – repeated indices are summed over

$$u_i v_i = u_1 v_1 + u_2 v_2 + u_3 v_3 = \underline{u} \cdot \underline{v}$$

$$\text{Note, no need for } \sum_{i=1}^{3}$$

  3) No indices ever appears more than twice on the same symbol groupings

Navier-Stokes in Index notation

- We can express the Navier-Stokes equations as follows

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}$$

Notice summation here. In 3D this becomes

$$\frac{\partial u_i}{\partial t} + u_1 \frac{\partial u_i}{\partial x_1} + u_2 \frac{\partial u_i}{\partial x_2} + u_3 \frac{\partial u_i}{\partial x_3} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \nu \left[\frac{\partial^2 u_i}{\partial x_1^2} + \frac{\partial^2 u_i}{\partial x_2^2} + \frac{\partial^2 u_i}{\partial x_3^2}\right]$$

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Questions 1

1) Identify if the following expressions are scalars, vectors or tensors

$$\underline{\nabla}\, C \qquad \underline{\nabla} \cdot \underline{u} \qquad \underline{\nabla}\, \underline{u} \qquad \frac{\partial \underline{u}}{\partial t} \qquad \underline{\nabla} \cdot \underline{\underline{\Pi}}$$

2) Write the expressions from 1) in index notation (u_1, u_2, u_3, x_1, x_2, x_3, Pi_{11}, Pi_{12}, etc).

3) Expand the vector form of the Navier-Stokes Equations to write in terms of u,v and w and x,y and z.

$$\frac{\partial \underline{u}}{\partial t} + \underline{u} \cdot \underline{\nabla}\, \underline{u} = -\frac{1}{\rho} \underline{\nabla} P + \nu \nabla^2 \underline{u}$$

Derivation of the Navier-Stokes Equation

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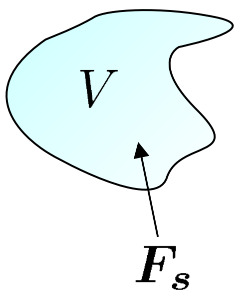
Newton's Second Law

$$m\frac{d^2\boldsymbol{r}}{dt^2} = \mathbf{F}$$

Newton's Second Law



$$m\frac{d^2\boldsymbol{r}}{dt^2} = \mathbf{F}$$

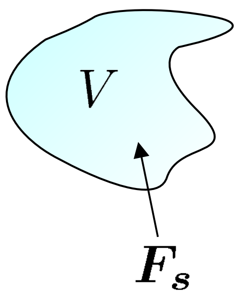
$$\frac{d}{dt}\int_V \rho \boldsymbol{u} dV = \boldsymbol{F}_s$$

Lagrangian

Newton's Second Law

$$m\frac{d^2\boldsymbol{r}}{dt^2} = \mathbf{F}$$

$$m_i\frac{d^2\boldsymbol{r}_i}{dt^2} = \boldsymbol{F}_i$$



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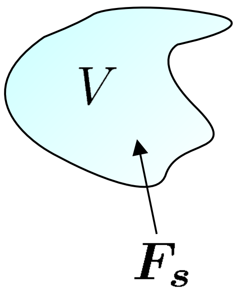
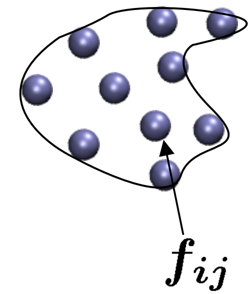




$$\frac{d}{dt}\int_V \rho\boldsymbol{u}dV = \boldsymbol{F}_s$$

Lagrangian

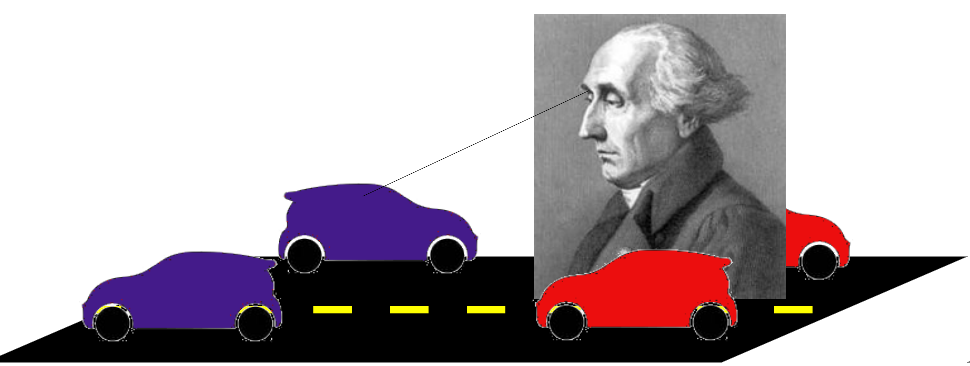
$$\frac{d}{dt}\sum_{i=1}^{N} m_i\frac{d\mathbf{r}_i}{dt} = \sum_{i=1}^{N}\sum_{j\neq i}^{N}\mathbf{f}_{ij}$$

Reference Frame

Lagrangian

Moves with the fluid parcel

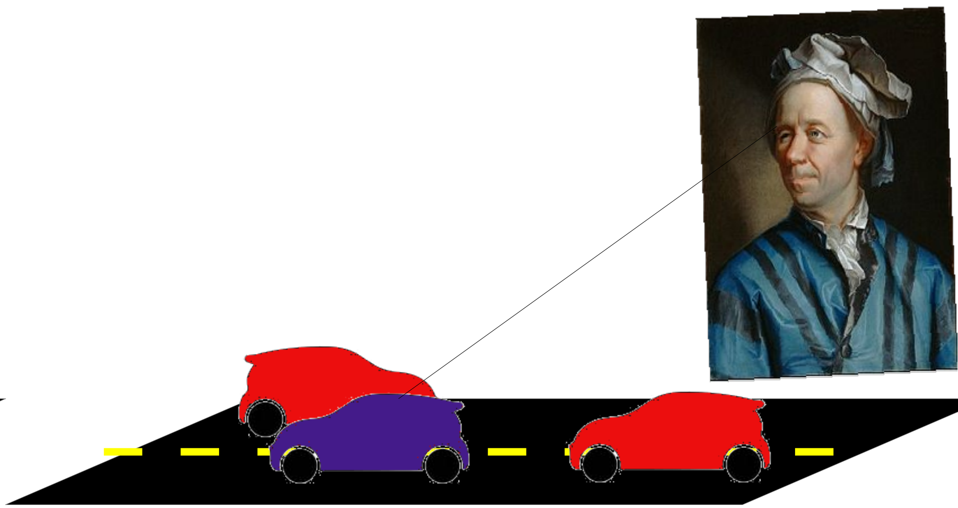
$$u = u(t)$$



Eulerian

Stays in one place and observes flow past

$$u = u(\underline{r}, t)$$



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Reference Frame

1) Reynold's Transport Theorem

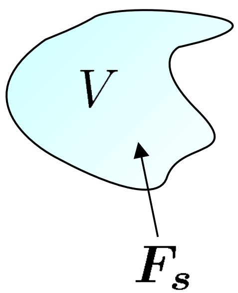
Relates the two frameworks

$$\frac{d}{dt}\int_{V(t)} \rho \underline{u} dV = \int_{V(t)} \frac{\partial}{\partial t} \rho \underline{u} dV + \oint_S \rho \underline{u}\underline{u} \cdot d\mathbf{S}$$

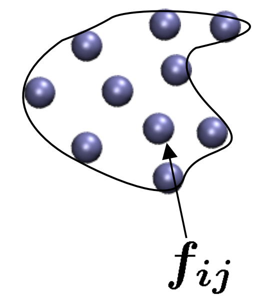
Because volume is a function of time in a Lagrangian framework, differentiation with respect to time gives an extra term using chain rule

This term measures how much momentum flows over the suface of a fixed volume (convection)

Newton's Second Law



$$m\frac{d^2\boldsymbol{r}}{dt^2} = \mathbf{F}$$



$$\frac{d}{dt}\int_V \rho \boldsymbol{u} dV = \boldsymbol{F}_s$$

Lagrangian

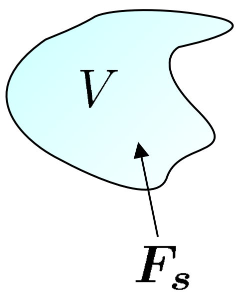
$$\frac{d}{dt}\sum_{i=1}^{N} m_i \frac{d\mathbf{r}_i}{dt} = \sum_{i=1}^{N}\sum_{j\neq i}^{N}\mathbf{f}_{ij}$$

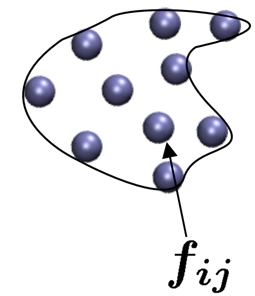
$$\int_V \frac{\partial}{\partial t}\rho \boldsymbol{u} dV + \oint \rho \boldsymbol{u}\boldsymbol{u} \cdot d\boldsymbol{S} = \boldsymbol{F}_s$$

Eulerian

Newton's Second Law

$$m\frac{d^2\boldsymbol{r}}{dt^2} = \mathbf{F}$$





$$\frac{d}{dt}\int_V \rho\boldsymbol{u}dV = \boldsymbol{F}_s$$

Lagrangian

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \frac{d\mathbf{r}_i}{dt} = \sum_{i=1}^{N}\sum_{j\neq i}^{N}\mathbf{f}_{ij}$$

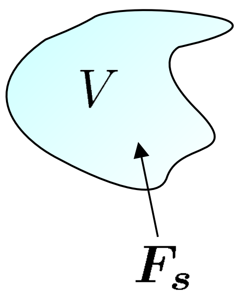
$$\int_V \frac{\partial}{\partial t}\rho\boldsymbol{u}dV + \int_V \boldsymbol{\nabla}\cdot\rho\boldsymbol{u}\boldsymbol{u}dV = \boldsymbol{F}_s$$

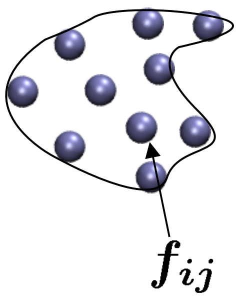
Eulerian

Divergence
theorem

Newton's Second Law

$$m\frac{d^2\boldsymbol{r}}{dt^2} = \mathbf{F}$$





$$\frac{d}{dt}\int_V \rho\boldsymbol{u}\,dV = \boldsymbol{F}_s$$

Lagrangian

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \frac{d\mathbf{r}_i}{dt} = \sum_{i=1}^{N}\sum_{j\neq i}^{N} \mathbf{f}_{ij}$$

$$\frac{\partial}{\partial t}\rho\boldsymbol{u} + \boldsymbol{\nabla}\cdot\rho\boldsymbol{u}\boldsymbol{u} = \boldsymbol{F}_s$$

Pointwise

Eulerian

$$\rho = \rho(\boldsymbol{r}, t)$$

$$\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{r}, t)$$

$$\boldsymbol{F}_s = \boldsymbol{F}_s(\boldsymbol{r}, t)$$

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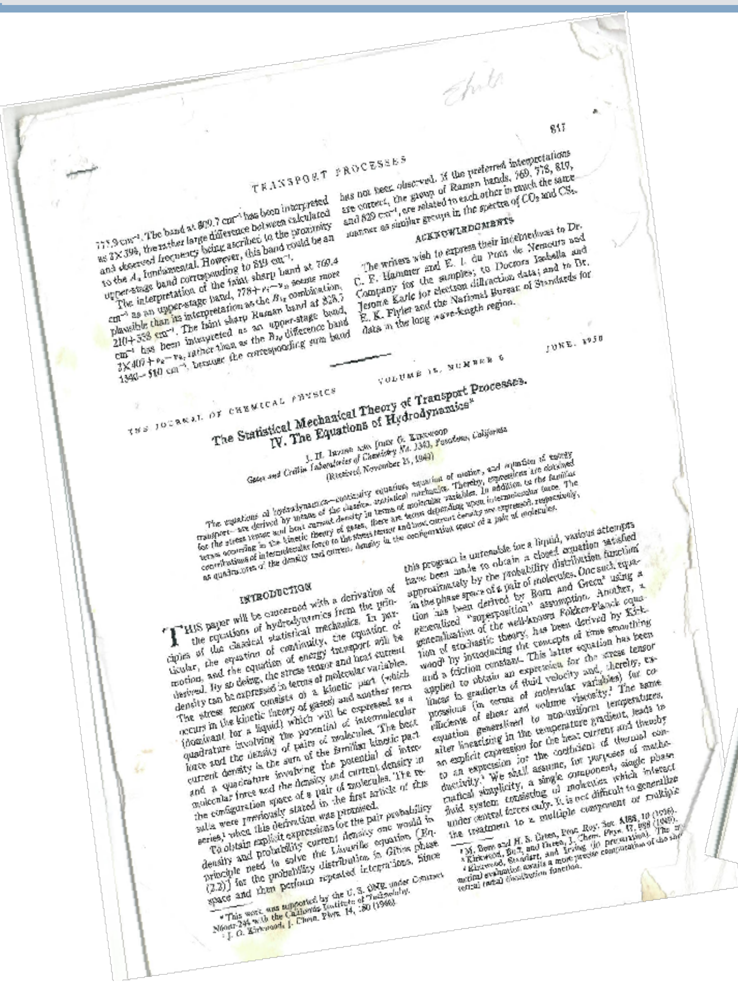
Irving and Kirkwood (1950)



THE JOURNAL OF CHEMICAL PHYSICS VOLUME 18, NUMBER 6 JUNE, 1950

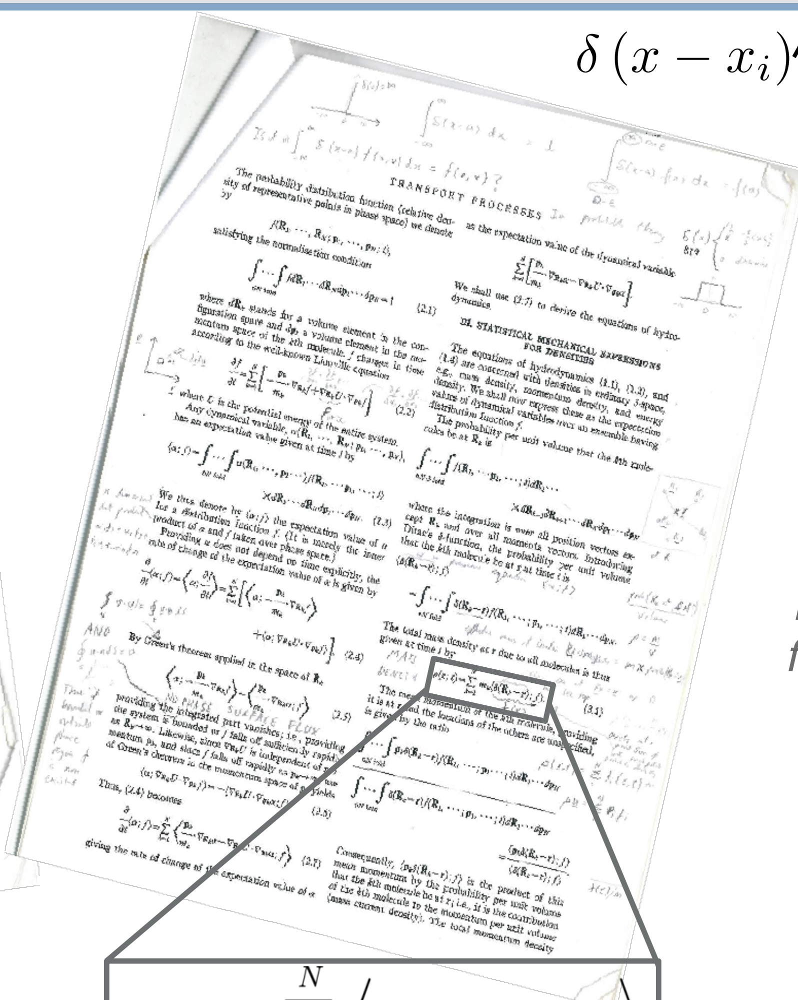
The Statistical Mechanical Theory of Transport Processes. IV. The Equations of Hydrodynamics*

J. H. Irving and John G. Kirkwood

Gates and Crellin Laboratories of Chemistry, California Institute of Technology, Pasadena, California

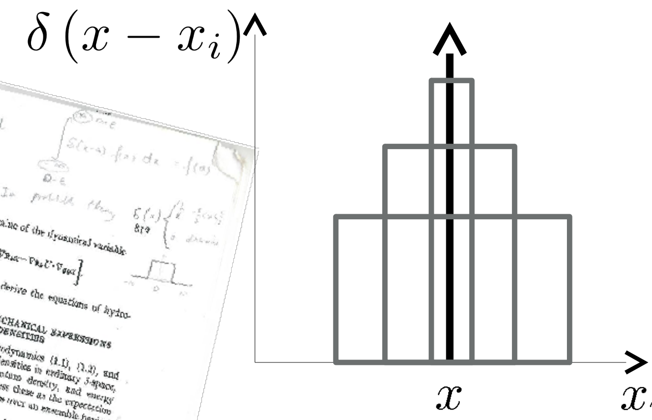
(Received November 21, 1949)

INTRODUCTION



TRANSPORT PROCESSES

III. STATISTICAL MECHANICAL EXPRESSIONS FOR DENSITIES



$$\rho(\boldsymbol{r},t)=\sum_{i=1}^{N}\left\langle m_i\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right);f\right\rangle$$

The Dirac delta infinitely high, infinitely thin peak formally equivalent to the continuum differential formulation

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The link to the Molecular System

Ensemble average and Dirac delta

1) Density

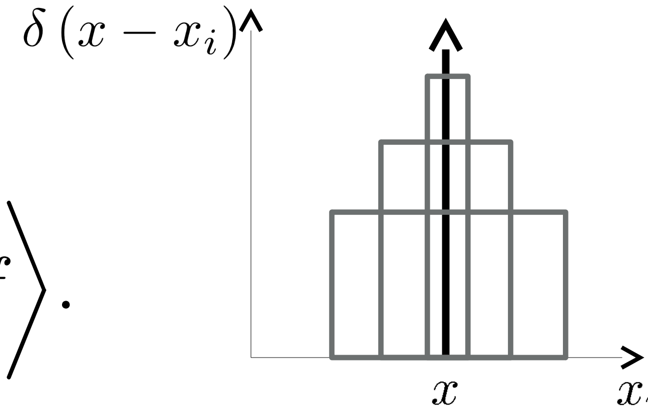
$$\rho(\boldsymbol{r},t) \equiv \sum_{i=1}^{N} \left\langle m_i \delta(\boldsymbol{r}_i - \boldsymbol{r}); f \right\rangle.$$

2) Momentum

$$\rho(\boldsymbol{r},t)\boldsymbol{u}(\boldsymbol{r},t) \equiv \sum_{i=1}^{N} \left\langle m_i \frac{d\boldsymbol{r}_i}{dt} \delta(\boldsymbol{r}_i - \boldsymbol{r}); f \right\rangle,$$

3) Temperature

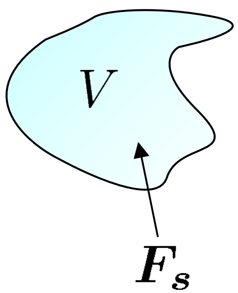
$$T(\boldsymbol{r},t) = \frac{1}{3k_B(N-1)} \sum_{i=1}^{N} \left\langle \left(\frac{d\boldsymbol{r}_i}{dt} - \boldsymbol{u} \right)^2 \delta(\boldsymbol{r}_i - \boldsymbol{r}); f \right\rangle.$$

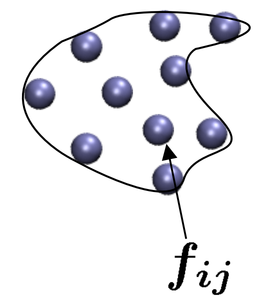


The Dirac delta infinitely high, infinitely thin peak formally equivalent to the continuum differential formulation

Newton's Second Law

$$m\frac{d^2\boldsymbol{r}}{dt^2} = \mathbf{F}$$





$$\frac{d}{dt}\int_V \rho \boldsymbol{u} dV = \boldsymbol{F}_s$$

Lagrangian

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \frac{d\mathbf{r}_i}{dt} = \sum_{i=1}^{N}\sum_{j\neq i}^{N} \mathbf{f}_{ij}$$

$$\frac{\partial}{\partial t}\rho\boldsymbol{u} + \boldsymbol{\nabla}\cdot\rho\boldsymbol{u}\boldsymbol{u} = \boldsymbol{F}_s$$

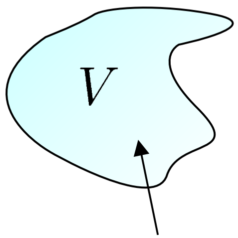
Pointwise Eulerian

$$\sum_{i=1}^{N}\left(\frac{d}{dt}m_i\dot{\mathbf{r}}_i + \boldsymbol{\nabla}\cdot m\mathbf{v}_i\mathbf{v}_i\right)\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right)$$
$$= \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}\mathbf{f}_{ij}\left[\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right) - \delta\left(\boldsymbol{r}-\boldsymbol{r}_j\right)\right]$$

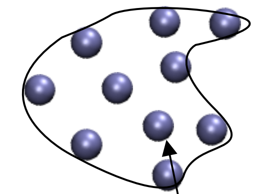
From Irving Kirkwood (1950)

Newton's Second Law

$$m\frac{d^2\boldsymbol{r}}{dt^2} = \mathbf{F}$$



$\boldsymbol{F}_s$



$\boldsymbol{f}_{ij}$

$$\frac{d}{dt}\int_V \rho \boldsymbol{u} dV = \boldsymbol{F}_s$$

Lagrangian

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \frac{d\mathbf{r}_i}{dt} = \sum_{i=1}^{N}\sum_{j\neq i}^{N} \mathbf{f}_{ij}$$

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Pointwise Eulerian

$$\sum_{i=1}^{N}\left(\frac{d}{dt}m_i\dot{\mathbf{r}}_i + \boldsymbol{\nabla}\cdot m\mathbf{v}_i\mathbf{v}_i\right)\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right)$$
$$= \frac{1}{2}\sum_{i=1}^{N}\sum_{j\neq i}^{N}\mathbf{f}_{ij}\left[\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right) - \delta\left(\boldsymbol{r}-\boldsymbol{r}_j\right)\right]$$

$$\frac{\partial}{\partial t}\rho\boldsymbol{u} = \boldsymbol{\nabla}\cdot\left[-\rho\boldsymbol{u}\boldsymbol{u} + \boldsymbol{\Pi}\right]_{CFD}$$

Pointwise Eulerian Stress

$$\sum_{i=1}^{N} m_i\ddot{\mathbf{r}}_i\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right) = \boldsymbol{\nabla}\cdot\left[-\rho\boldsymbol{u}\boldsymbol{u} + \boldsymbol{\Pi}\right]_{MD}$$

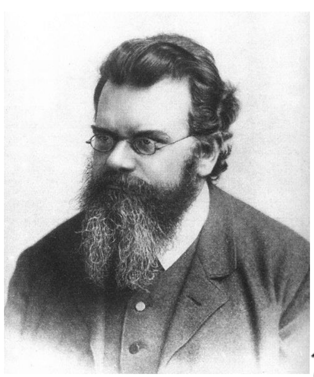
Molecular Pressure

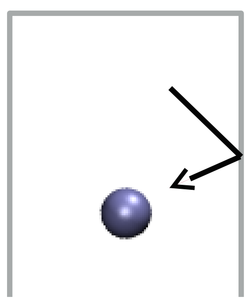
- Pressure in dense molecular systems have a long history
  - Virial form given by Rudolf Clausius in 1870
  - Irving and Kirkwood (1950) gave a full localised description,

$$\oint_S \mathbf{\Pi} \cdot d\mathbf{S} = \underbrace{\sum_{i=1}^{N} \left\langle \frac{\boldsymbol{p}_i \boldsymbol{p}_i}{m_i} \cdot d\mathbf{S}_i \right\rangle}_{\text{Kinetic}} + \underbrace{\frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \left\langle \boldsymbol{f}_{ij} \mathbf{n} \cdot d\mathbf{S}_{ij} \right\rangle}_{\text{Configurational}}$$

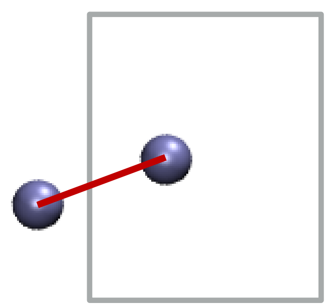
Kinetic theory part

Momentum due to average of molecules crossing a plane and returning





$$\dot{r}_i = \frac{p_i}{m_i} + u$$



Configurational part

Inter-molecular bonds act like the stress in a stretched spring

Simplifying The Pressure Term

- In the continuum, we do not have a way to get the pressure tensor. So we need to make some assumptions. First, split into thermodynamic pressure and a shear stress

$$\underline{\underline{\Pi}} = -P\underline{\underline{I}} + \underline{\underline{\tau}} = -P\delta_{ij} + \tau_{ij}$$

- Assume Linear stress strain-rate relationship (Newtonian fluid/no shear thinning)

$$\tau_{ij} \approx C_{ijkl}\epsilon_{kl}$$

$$\text{where } \epsilon_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right] = \frac{1}{2}\left[\underline{\nabla}\,\underline{u} + \underline{\nabla}\,\underline{u}^T\right]$$

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Simplifying The Pressure Term

- Assume an Isotropic fluid (81 components reduced to 2)

$$\tau_{ij} = C_{ijkl}\epsilon_{kl} = \lambda\epsilon_{kk}\delta_{ij} + 2\mu\epsilon_{ij}$$

- Two coefficients reduced to one using Stokes' hypothesis (note viscosity coefficient is assumed to be homogeneous so constant in all domain)

$$3\lambda + 2\mu = 0 \qquad \tau_{ij} = -\frac{2}{3}\mu\epsilon_{kk}\delta_{ij} + 2\mu\epsilon_{ij}$$

- Incompressible assumption allows further simplification

$$\underline{\nabla} \cdot \underline{u} = \frac{\partial u_i}{\partial x_i} = 0 \qquad \tau_{ij} = 2\mu\epsilon_{ij} \qquad \frac{\partial \tau_{ij}}{\partial x_j} = \mu\nabla^2 u_i$$

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Simplifying The Pressure Term

- So the final form the pressure tensor used in the Navier Stokes Equations is,

$$\frac{\partial}{\partial x_j}\Pi_{ij} = -\frac{\partial P}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j \partial x_j} = -\underline{\nabla} P + \mu \nabla^2 \underline{u}$$

- We have a single coefficient of viscosity. This is the coefficient obtain from molecular dynamics using auto-correlation functions (Green-Kubo)

$$\mu = \frac{V}{k_b T} \int_0^\infty \Big\langle \tau_{xy}(t) \tau_{xy}(0) \Big\rangle dt$$

The Navier-Stokes Equation

- Describes the flow of single phase Newtonian fluids

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

Note, left hand side has been expanded by assuming incompressibility and both sides divided by density

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Summary of Assumptions

- Newtonian framework (non-relatavistic and classical)
- Fields are continuous (continuum hypothesis)
- For constitutive laws
  - Stress is a linear function of Strain rate
  - Isotropy of fluid
  - Stoke's hypothesis
  - Viscosity coefficient is homogeneous
  - Usually Incompressiblity as well
- Structure of the molecules replaced with a mean field approach
- Viscosity models how quickly flow occurs, autocorrelation in an MD system can get viscosity - a model parameter in the continuum assumed constant as MD on much shorter times.
- A continuum system will reproduce the behaviour of billions of molecules over long times for relatively little computation effort

Limitations and Extensions

- Only considered single phase flows, we need to model an interface; nucleation, contact lines and phase change are also very difficult to model
- No model for energy, a separate equation solved if required
- High speed flows (high Mach number) require compressibility to be modelled
- Turbulence requires very large scale simulations and possibility additional models
- Flow through porous or granular material more complex
- Non-Newtonian fluid require complex visco-elastic behaviour through additional models
- Even simple models are often too expensive and complex to be used as as part of a general plant scale optimisation

Break

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Summary of the Origin of Terms

Kinematic viscosity is dynamic viscosity divided by density $\nu \equiv \frac{\mu}{\rho}$

$$\underbrace{\frac{\partial \underline{u}}{\partial t} + \underline{u} \cdot \underline{\nabla}\, \underline{u}}_{\text{Acceleration in Eulerian Reference Frame}} = \underbrace{-\frac{1}{\rho}\underline{\nabla} P + \nu \nabla^2 \underline{u}}_{\text{Force, written as divergence of pressure tensor and then split into scalar pressure and strain times viscosity coefficient}}$$

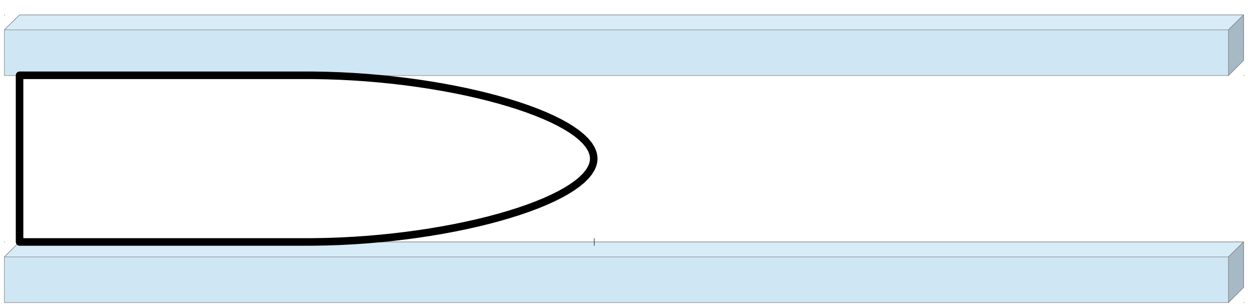
Acceleration in Eulerian Reference Frame

Force, written as divergence of pressure tensor and then split into scalar pressure and strain times viscosity coefficient

Simplifying the Navier-Stokes Equation

- Often we don't need all the terms, for example consider pressure driven flow between wide parallel plates

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



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Simplifying the Navier-Stokes Equation

Assume no convection (fully developed) 0

Assume pressure gradient is constant in x, zero in all other directions $\frac{\partial P}{\partial x}$

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

Assume wide channel so 2D

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

Simplifying the Navier-Stokes Equation

Taking only the x component of velocity

$$\underbrace{\frac{\partial u}{\partial t}}_{\substack{\textbf{Unsteady}\\\textbf{Term}}} = \nu \underbrace{\left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right]}_{\substack{\textbf{Diffusion}\\\textbf{Equation}}} - \underbrace{\frac{1}{\rho}\frac{\partial P}{\partial x}}_{\substack{\textbf{Constant}\\\textbf{Pressure}\\\textbf{Term}}}$$

Review of Numerical Methods

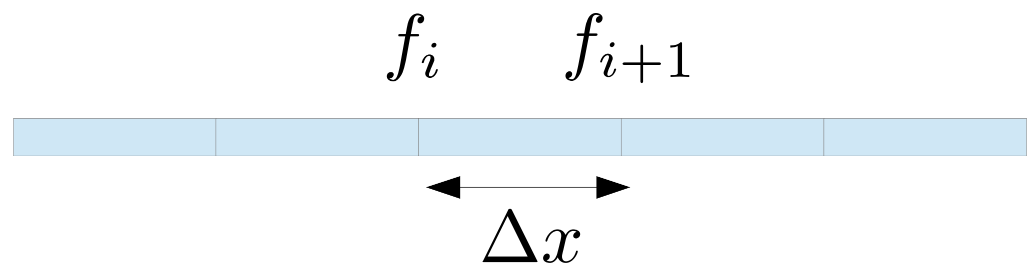
Numerical Solution to Differential Equations

- 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

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



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
```

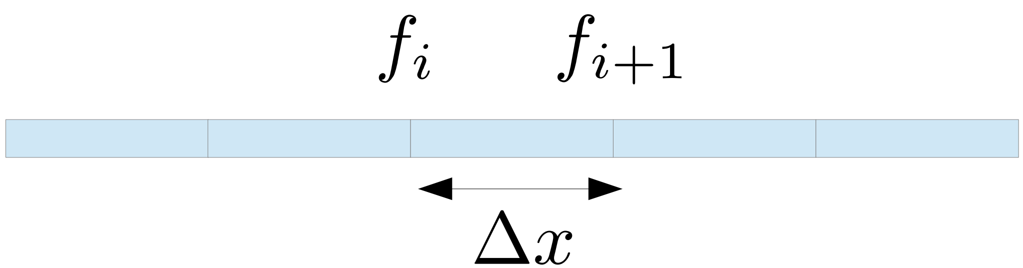
$$\frac{d^2 f}{dx^2} = b$$

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

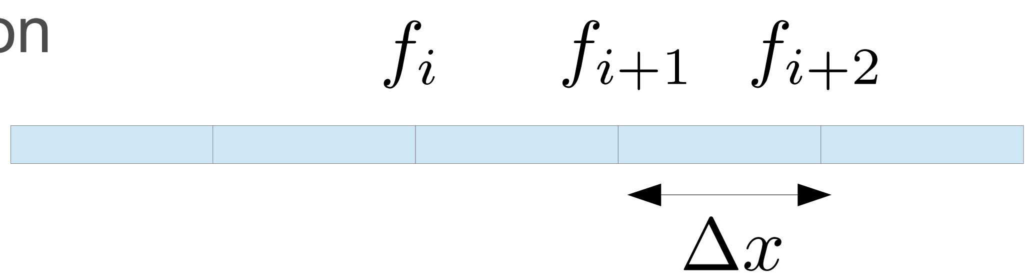
Numerical Solution to Differential Equations

- 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



Solving Partial Equations Numerically

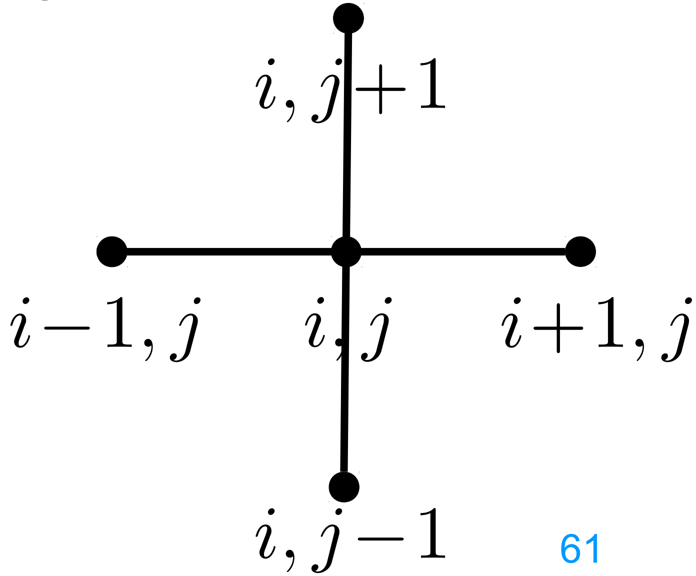
- The same concept can be applied in two dimensions

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

- Using cell indices, derivatives in each direction can be seen to use what is called a five point "stencil"

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

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



Solve this Equation

$$\underbrace{\frac{\partial u}{\partial t}}_{\text{Unsteady Term}} = \nu \left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right] - \frac{1}{\rho} \underbrace{\frac{\partial P}{\partial x}}_{\text{Constant Pressure Term}}$$

Diffusion Equation

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Solve this Equation

- The only new term is the time evolution, which is evaluated as follows

$$\frac{\partial u}{\partial t} \approx \frac{u(t+\Delta t) - u(t)}{\Delta t} = \frac{u_{i,j}^{n+1} - u_{i,j}^{n}}{\Delta t}$$

- The evolution in time is denoted by superscripts where the spatial location is still denoted by subscripts

$$\frac{u_{i,j}^{n+1} - u_{i,j}^{n}}{\Delta t} = \nu \left[\frac{u_{i+1,j}^{n} - 2u_{i,j}^{n} + u_{i-1,j}^{n}}{(\Delta x)^2} + \frac{u_{i,j+1}^{n} - 2u_{i,j}^{n} + u_{i,j-1}^{n}}{(\Delta y)^2} \right] - \frac{1}{\rho}\frac{\partial P}{\partial x}$$

Solve this Equation

- Starting from this equation

$$\frac{u_{i,j}^{n+1}-u_{i,j}^{n}}{\Delta t}=\nu\left[\frac{u_{i+1,j}^{n}-2u_{i,j}^{n}+u_{i-1,j}^{n}}{(\Delta x)^2}+\frac{u_{i,j+1}^{n}-2u_{i,j}^{n}+u_{i,j-1}^{n}}{(\Delta y)^2}\right]-\frac{1}{\rho}\frac{\partial P}{\partial x}$$

- We rearrange to get the next time step as follows

$$u_{i,j}^{n+1}=u_{i,j}^{n}+\Delta t\frac{\mu}{\rho}\left[\frac{u_{i+1,j}^{n}-2u_{i,j}^{n}+u_{i-1,j}^{n}}{(\Delta x)^2}+\frac{u_{i,j+1}^{n}-2u_{i,j}^{n}+u_{i,j-1}^{n}}{(\Delta y)^2}\right]-\frac{\Delta t}{\rho}\frac{\partial P}{\partial x}$$

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Example MATLAB Script

```
%problem definition
mu = 10e-3;
rho = 1000.0;
nu = mu/rho;

%Constants
Npoints = 10;
Lx = 1.0;
Ly = 1.0;
dx = Lx/(Npoints-1);
dy = Ly/(Npoints-1);
dt = 10.0;
dPdx = 1.0;
u = zeros(Npoints,Npoints);
un = zeros(Npoints,Npoints);

%Analytical solution
y = linspace(0.0, Ly, Npoints);
uanaly = 0.5*(dPdx/mu)*(y.^2-Ly*y);
```

```
for it =1:10000
    %Loop over all points
    for j=2:Npoints-1
        for i=2:Npoints-1
            un(i,j) = u(i,j) + dt*nu* ...
                    ((u(i+1,j)-2.0*u(i,j)+u(i-1,j))/dx^2 ...
                    +(u(i,j+1)-2.0*u(i,j)+u(i,j-1))/dy^2) ...
                    -dt*dPdx/rho;
        end
    end
    u = un;
    %Enforce Boundary Condition
    u(:,1) = 0.0; %Bottom Wall Boundary
    u(1,:) = u(end-1,:); %Left periodic BC
    u(end,:) = u(2,:); %Right periodic BC
    u(:,end) = 0.0; %Top Wall Boundary
    %Plotting
    plot(y, u(5,:), '-o'); hold all
    plot(y, uanaly, 'r-'); hold off
    pause(0.001)
end
```

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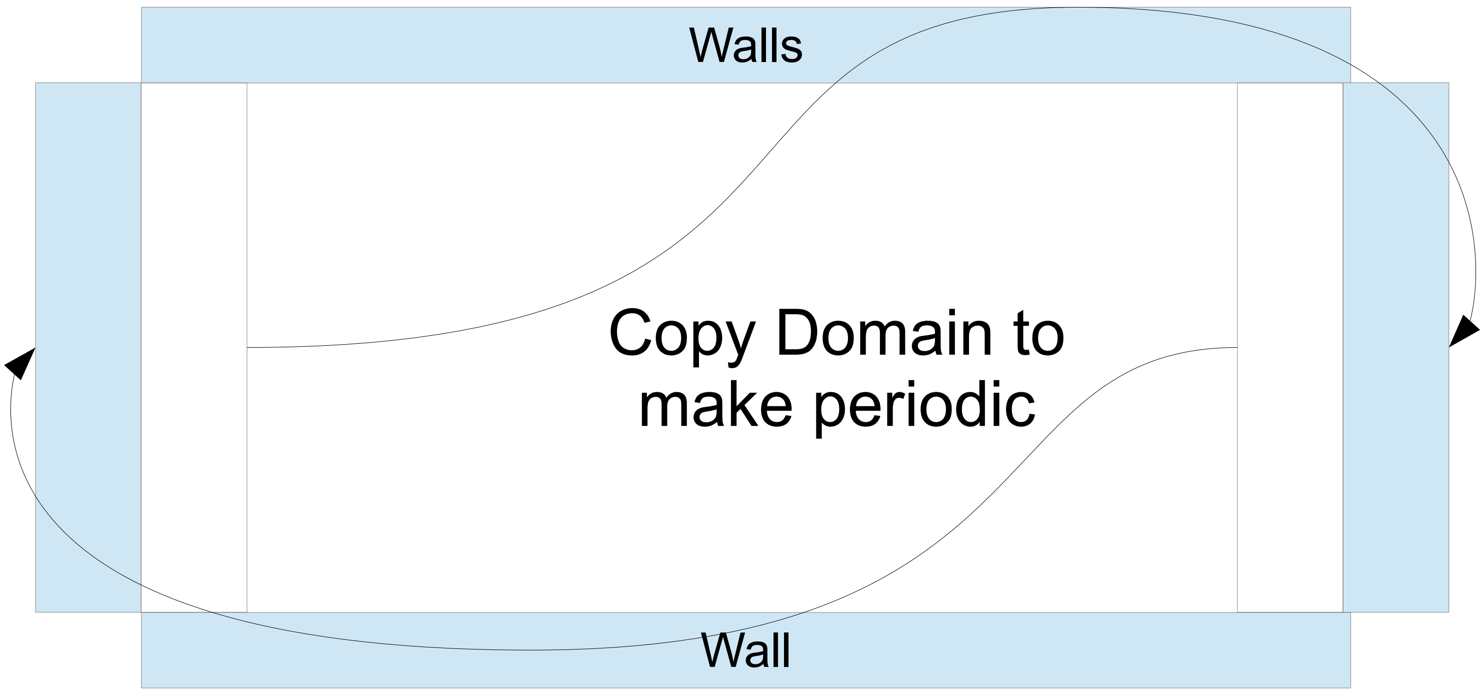
Boundary Conditions



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