Imperial College London

Brunel University London

A Tutorial of Boiling Simulation using Coupled Molecular Dynamics and Computational Fluid Dynamics

Royal Society-DFID

Africa Capacity Building Initiative

19th July

Edward Smith

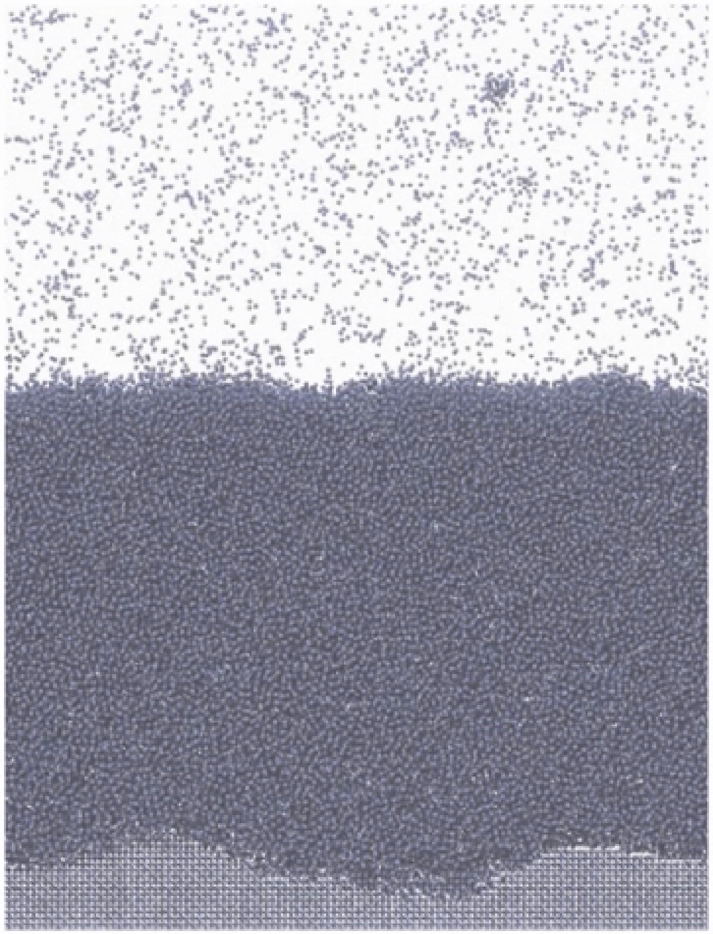
Plan

- Introductions to Computational Fluid Dynamics (CFD)
  - Assumptions and modelling paradigm
  - Introduction to numerical solutions
- Hands on 1
- Introductions to Molecular Dynamics (MD)
  - Assumptions and modelling paradigm
  - Introduction to numerical solutions
- Coupled Simulation
- Hands on 2

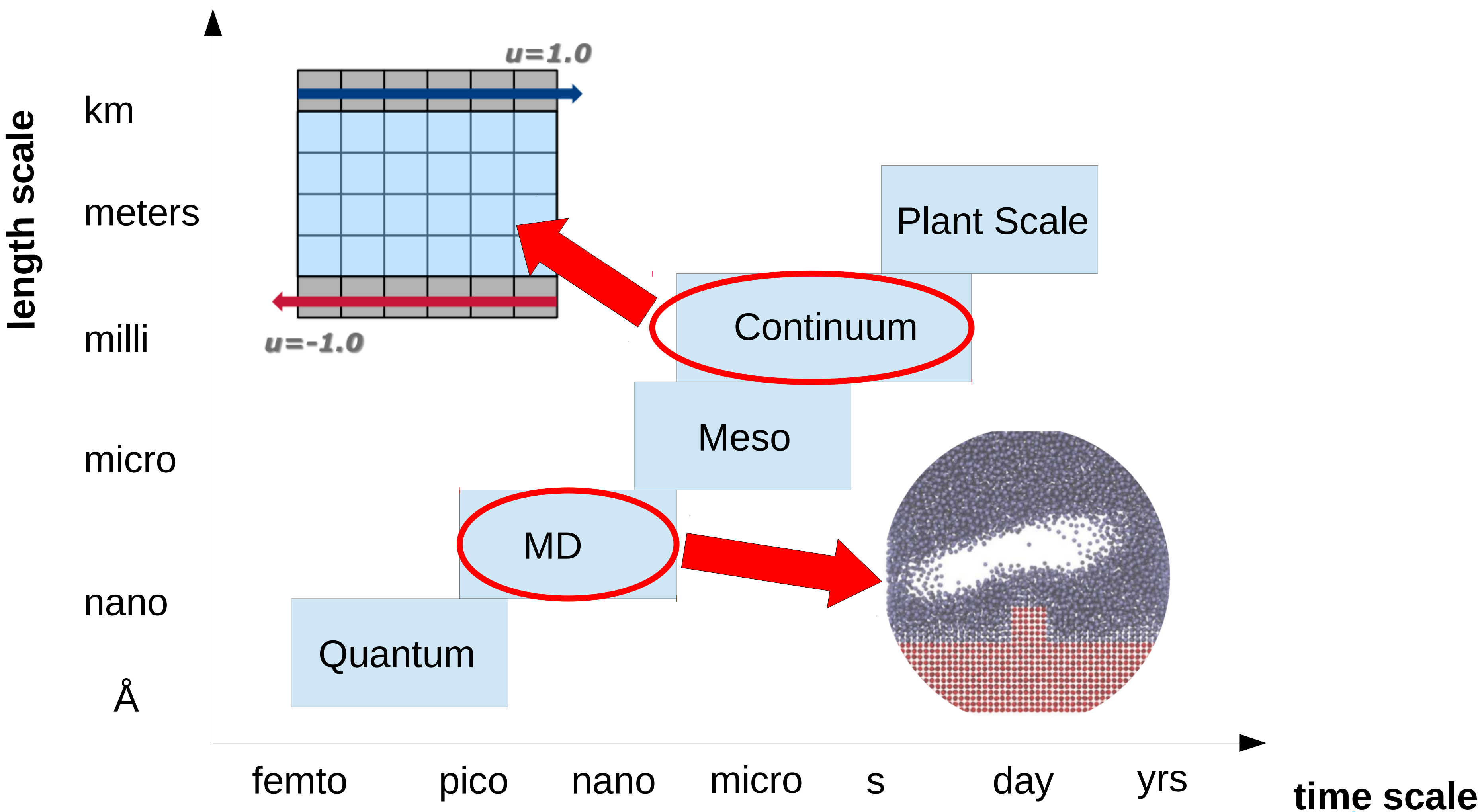
Slides and hands-on code at

edwardsmith.co.uk/content/RS-DFID.zip

Molecular Dynamics (MD)

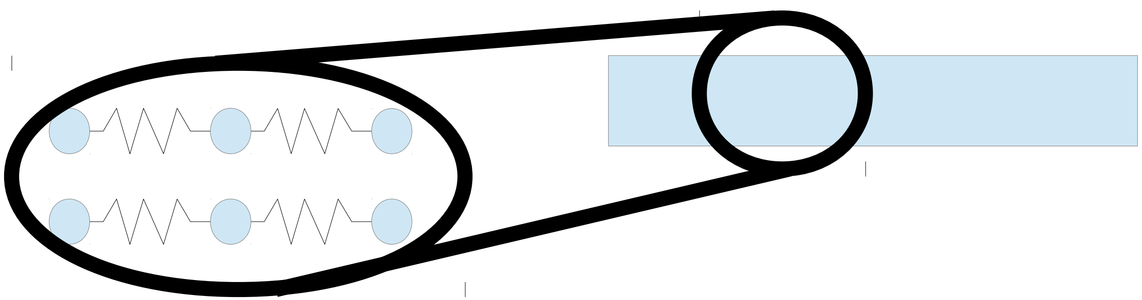


Scale Hierarchy



Continuum Fields

- The continuum hypothesis refers to continuous fields in space
- Assumes so many particles that a substance is continuous.



- In practice, one meter cube of air has 10^{25} molecules so works very well in almost any case on interest
- A typical MD simulation may have ~10^4 molecules which is nanometer scale - bigger than micrometer is prohibitive
- You should always use the simplest/cheapest model that captures the physics of interest
- A continuum system will reproduce the behaviour of countless molecules for relatively little computation effort

The Navier-Stokes Equation

- Describes the flow of continuum fluid

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

- A non-linear partial-differential velocity and pressure equation
- Cannot solve directly and not proven to have existence and smoothness (Clay prize with $1,000,000 reward)
- We will aim to solve numerically today

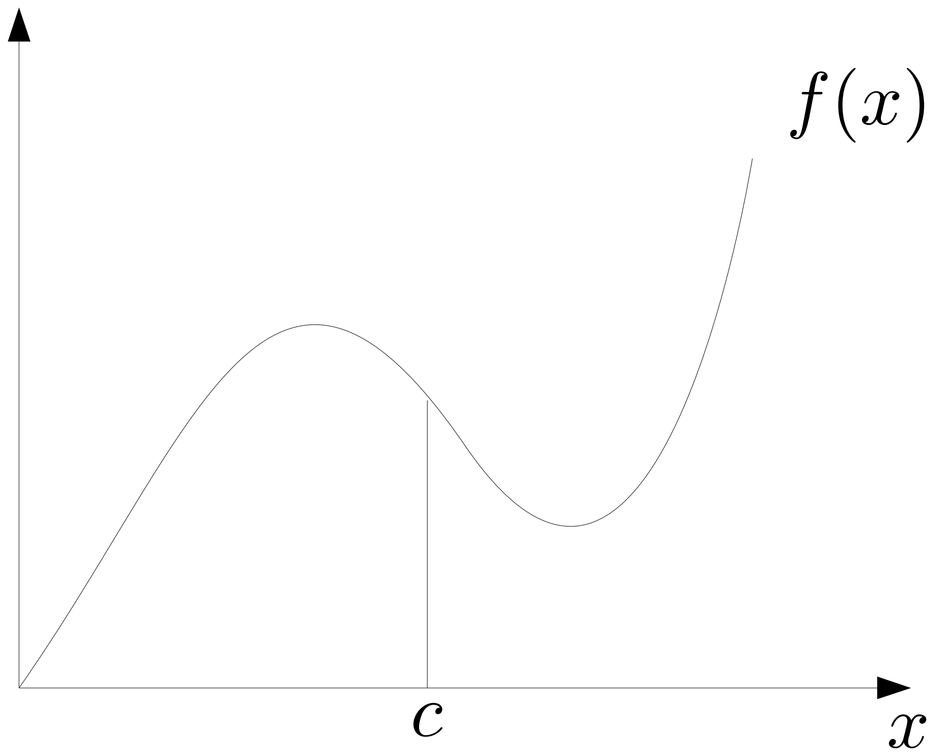
Summary of Assumptions

- Newtonian framework (non-relatavistic and classical)

- For constitutive laws
  - Stress is a linear function of Strain rate
  - Isotropy of fluid
  - Stoke's hypothesis
  - Viscosity coefficient is homogeneous
  - Usually Incompressiblity assumed as well

- Structure of the molecules replaced with a continuous mean field (the continuum hypothesis)

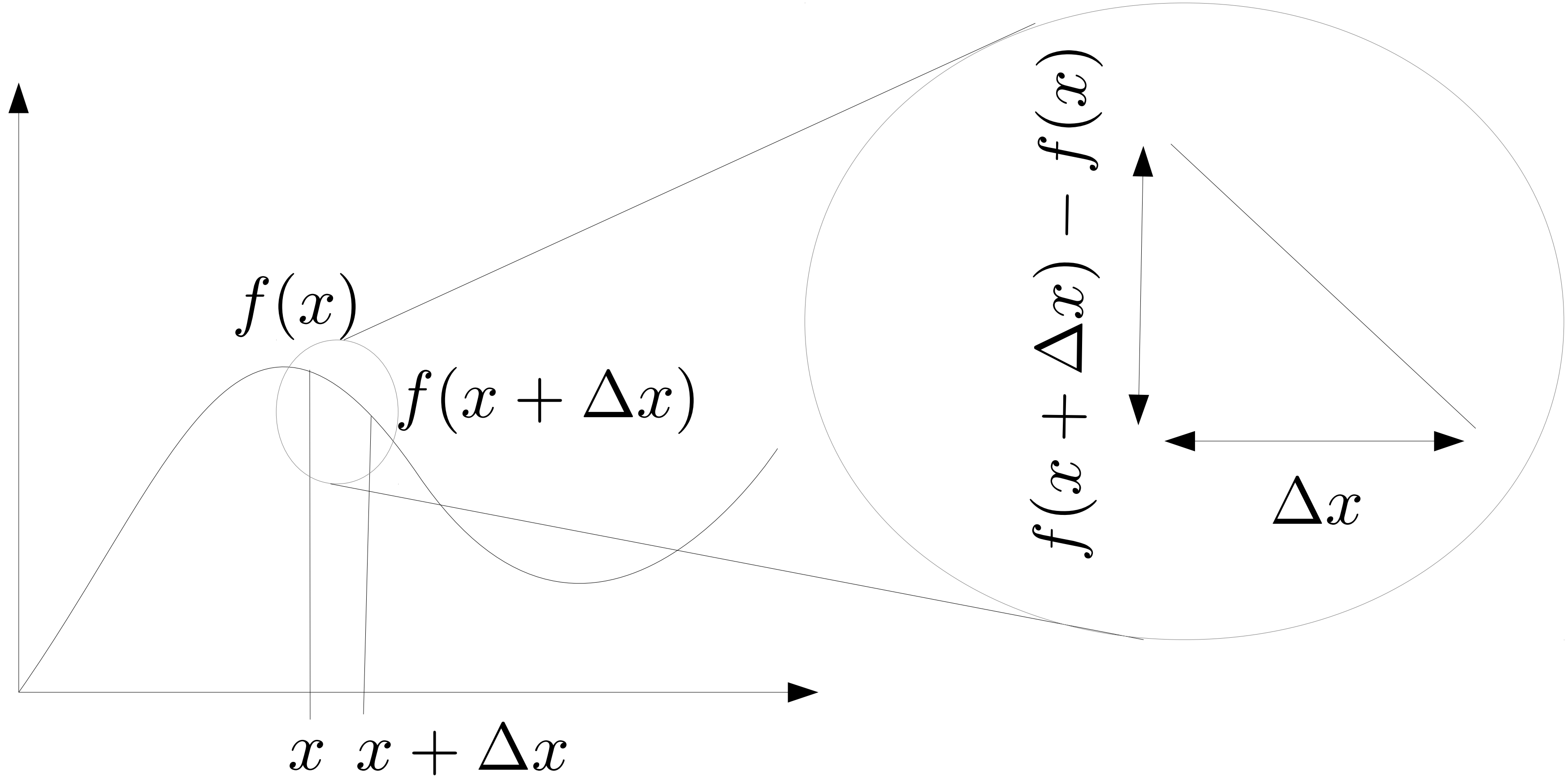
Definition of a Continuous Function



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

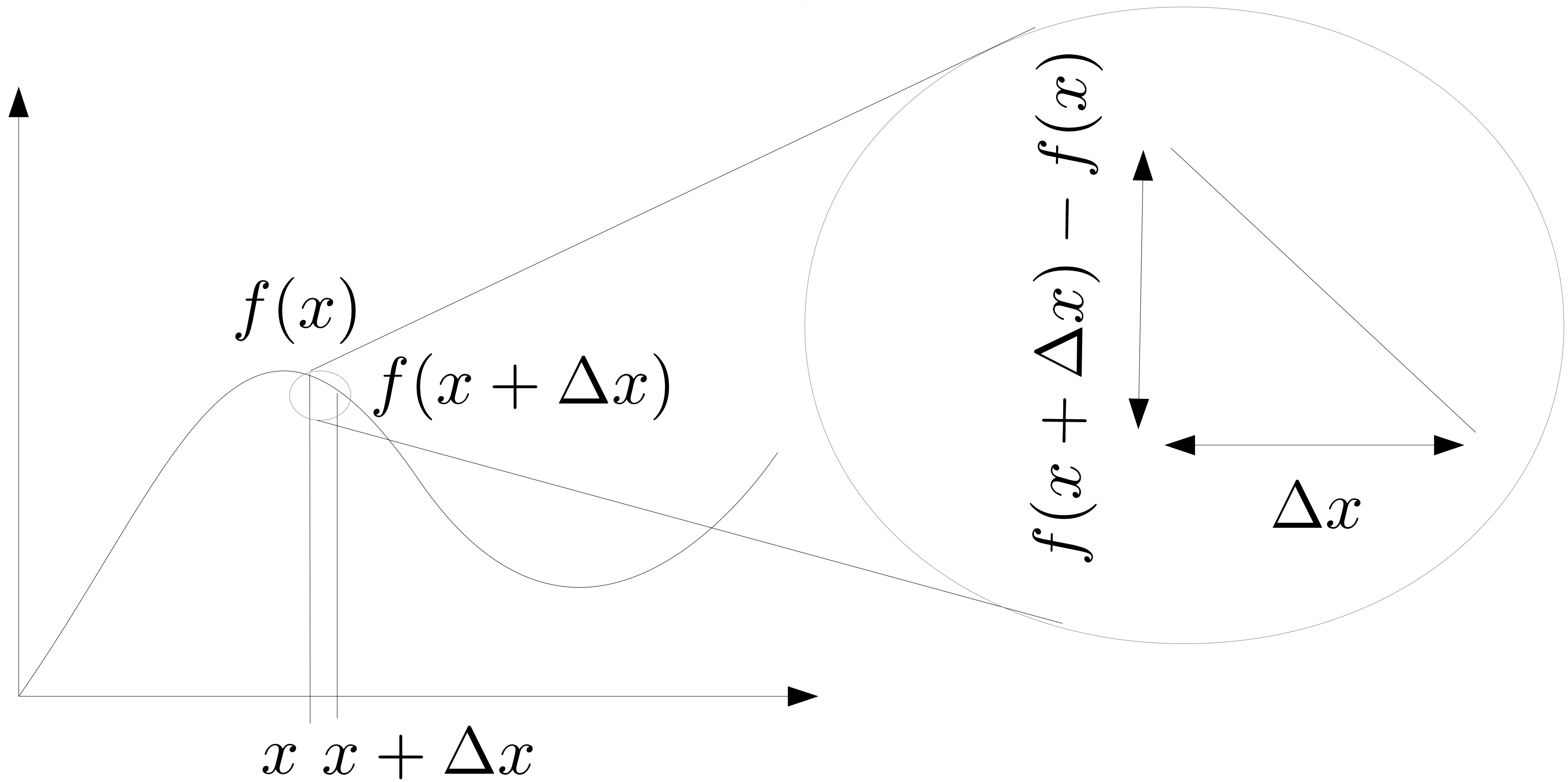
Also $\epsilon - \delta$ definition which is more formal.

Definition of a Derivative



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

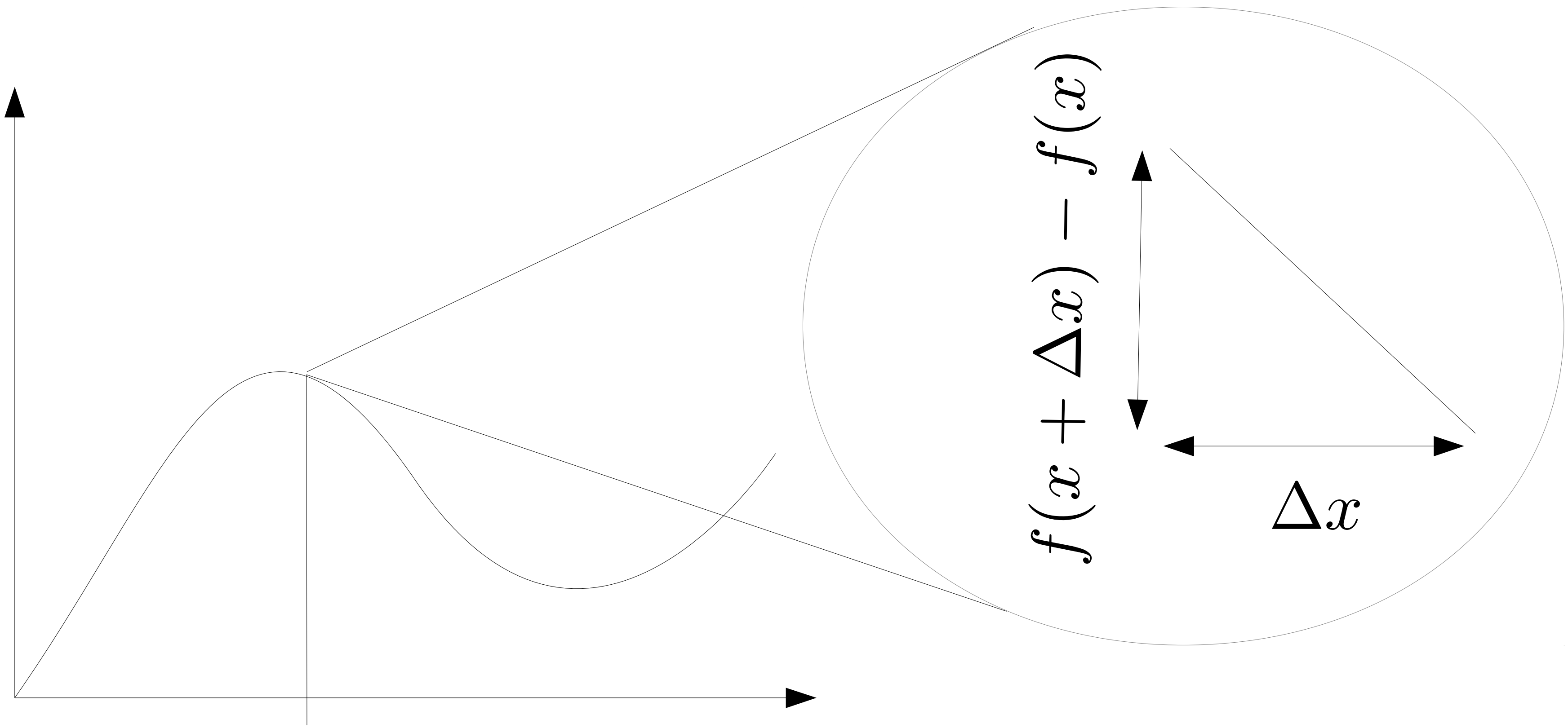
Definition of a Derivative



Better with smaller Δx

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

Definition of a Derivative



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

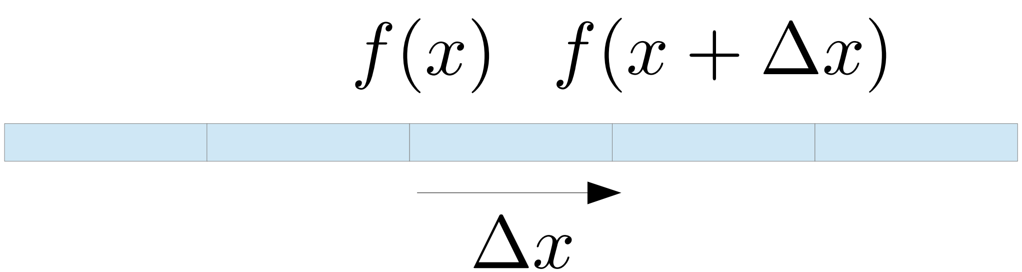
Numerical Solution to Differential Equations

- To 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

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

- Which we can write as code (rearranged to get i+1 value)

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

```
f(i+1) = f(i) + a*dx
```

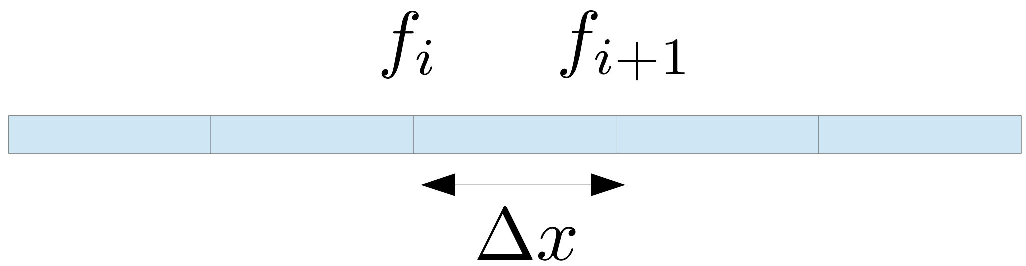
$$\frac{d^2 f}{dx^2} = b$$

```
f(i+1) = 2*f(i) - f(i-1) + b*dx**2
```

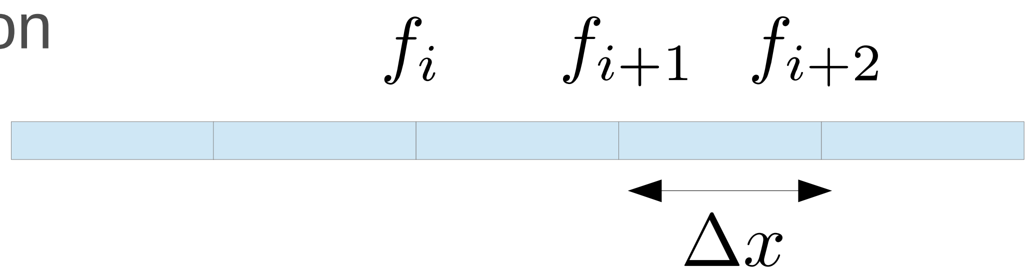
Numerical Solution to Differential Equations

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

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



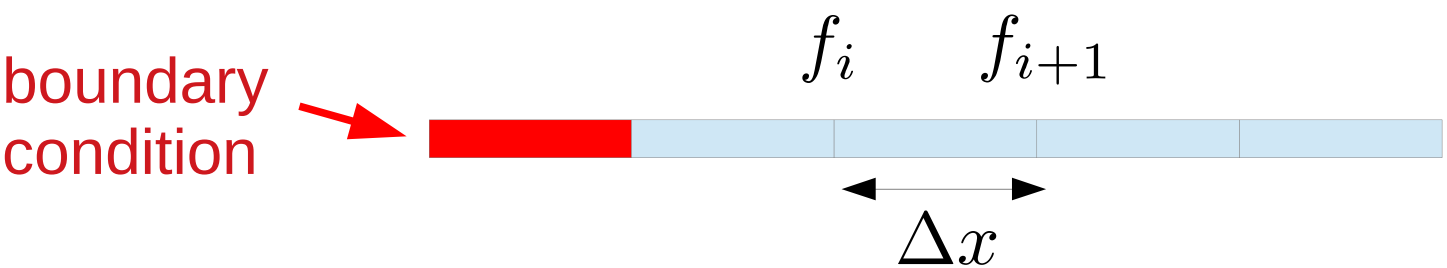
- Once we know the value at f_{i+1}, we can get the value at at f_{i+2}, and so on



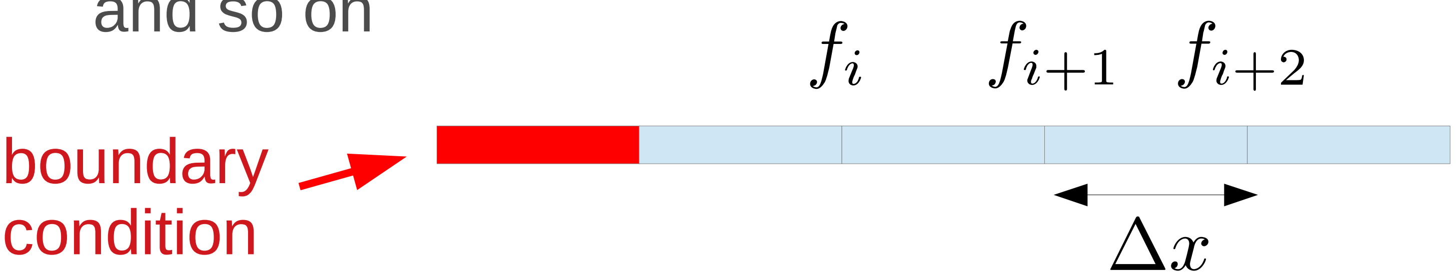
Boundary Conditions

- We need to specify one value, called a boundary condition, in order to solve this

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



- Boundar condition at f_0 determines all value at at f_i, f_{i+1}, f_{i+2} and so on



Functions of Time and Space

- Consider the unsteady diffusion equation

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} \qquad u = u(x,t)$$

- We have both a first order time derivative (unsteady term)

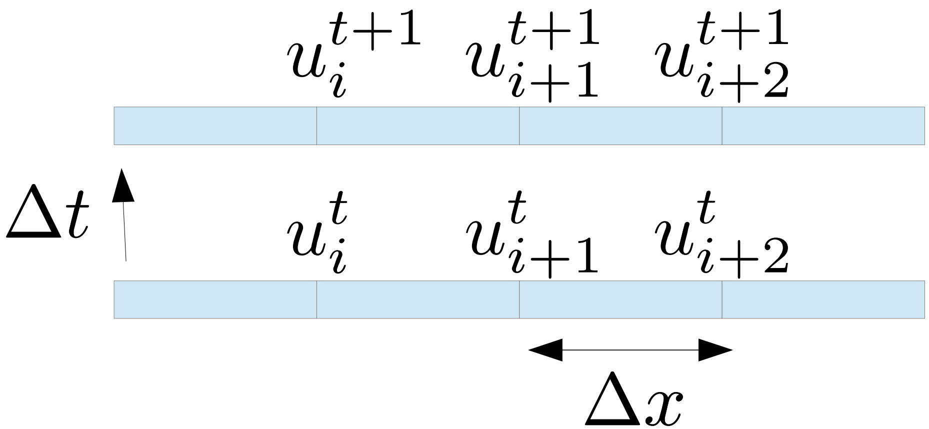
$$\frac{du}{dt} \approx \frac{u(x, t+\Delta t) - u(x,t)}{\Delta t} = \frac{u_i^{t+1} - u_i^t}{\Delta t}$$

- and the second order space derivative (diffusion term)

$$\frac{d^2u}{dx^2} \approx \frac{u_{i+1}^t - 2u_i^t + u_{i-1}^t}{(\Delta x)^2}$$

Functions of Time and Space

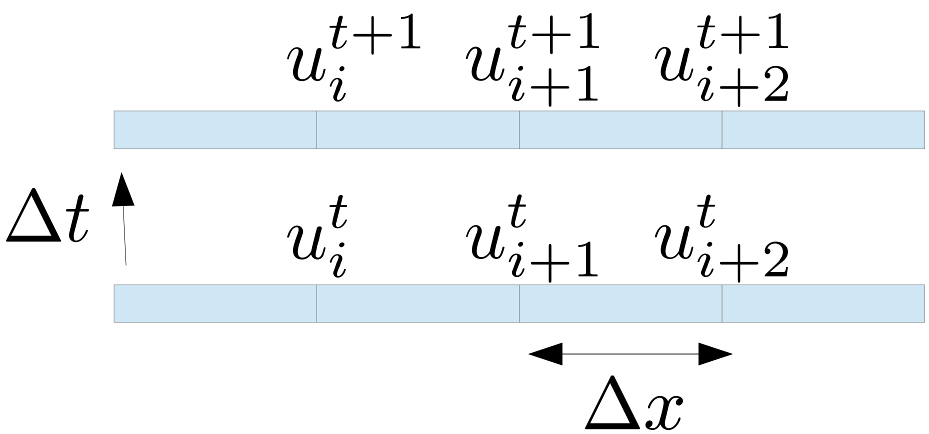
- Take each value at time t and calculate the field at the next time



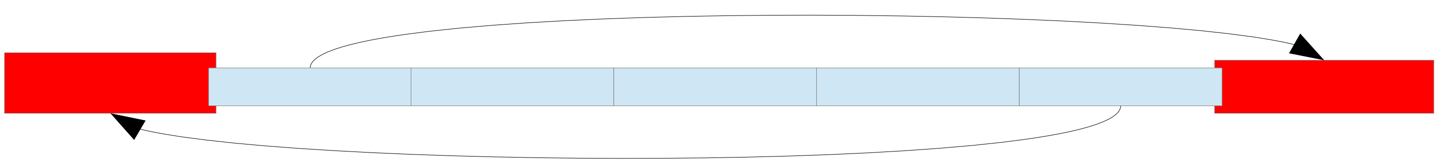
$$u_i^{t+1} = u_i^t + \Delta t \nu \left[\frac{u_{i+1}^t - 2u_i^t + u_{i-1}^t}{(\Delta x)^2} \right]$$

Functions of Time and Space

- Take each value at time t and calculate the field at the next time



- For simplicity, we use periodic boundaries



Copy Domain to make periodic

Full Navier Stokes (NS) in 1D

- Solving the Navier Stokes proceeds in the same way

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = -\frac{1}{\rho}\frac{\partial P}{\partial x} + \nu\frac{\partial u^2}{\partial x^2}; \quad \frac{\partial u}{\partial x} = 0$$

Pressure Term

Mass Continuity

$$\frac{u_i^{t+1} - u_i^t}{\Delta t}$$

Unsteady Term

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

Convection Term

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

Diffusion Term

Full Navier Stokes (NS) in 1D

- However we have two unknowns (u and P)

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = -\frac{1}{\rho}\frac{\partial P}{\partial x} + \nu\frac{\partial u^2}{\partial x^2}; \quad \frac{\partial u}{\partial x} = 0$$

$$\frac{u_i^{t+1} - u_i^t}{\Delta t} = \frac{u_i^{t+1} - u_i^*}{\Delta t} + \frac{u_i^* - u_i^t}{\Delta t}$$

Unsteady Term

Split time evolution into two stages and use mass continuity equation as second equation to solve for pressure

Solving for Pressure

- Split time integration into two stages

Unsteady Term

Convection Term

Diffusion Term

$$
\begin{cases}
\dfrac{u_i^* - u_i^t}{\Delta t} = -u\dfrac{\partial u}{\partial x} - \nu\dfrac{\partial u^2}{\partial x^2} \\[2ex]
\dfrac{u_i^{t+1} - u_i^*}{\Delta t} = -\dfrac{1}{\rho}\dfrac{\partial P}{\partial x}
\end{cases}
$$

Pressure Term

Solving for Pressure

- Split time integration into two stages and use mass continuity equation

Convection Term

Diffusion Term

Unsteady Term

$$\begin{cases} \dfrac{u_i^* - u_i^t}{\Delta t} = -u\dfrac{\partial u}{\partial x} - \nu\dfrac{\partial u^2}{\partial x^2} \\[2ex] \dfrac{\dfrac{\partial u_i^{t+1}}{\partial x} - \dfrac{\partial u_i^*}{\partial x}}{\Delta t} = -\dfrac{1}{\rho}\dfrac{\partial^2 P}{\partial x^2} \end{cases}$$

Mass Continuity =0

Pressure Term

Solving for Pressure

- Split time integration into two stages and use mass continuity equation

Unsteady Term

Convection Term

Diffusion Term

$$\begin{cases} \dfrac{u_i^* - u_i^t}{\Delta t} = -u\dfrac{\partial u}{\partial x} - \nu\dfrac{\partial u^2}{\partial x^2} \\ \dfrac{1}{\Delta t}\dfrac{\partial u_i^*}{\partial x} = \dfrac{1}{\rho}\dfrac{\partial^2 P}{\partial x^2} \end{cases}$$

Pressure Term

$$\frac{P_{i+1} - 2P_i + P_{i-1}}{(\Delta x)^2}$$

Also Python jupyter notebook at
edwardsmith.co.uk/content/Fluid_Dynamics_On_A_Line

Full Navier Stokes Solver in 1D

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = -\frac{1}{\rho}\frac{\partial P}{\partial x} + \nu\frac{\partial u^2}{\partial x^2}; \quad \frac{\partial u}{\partial x} = 0$$

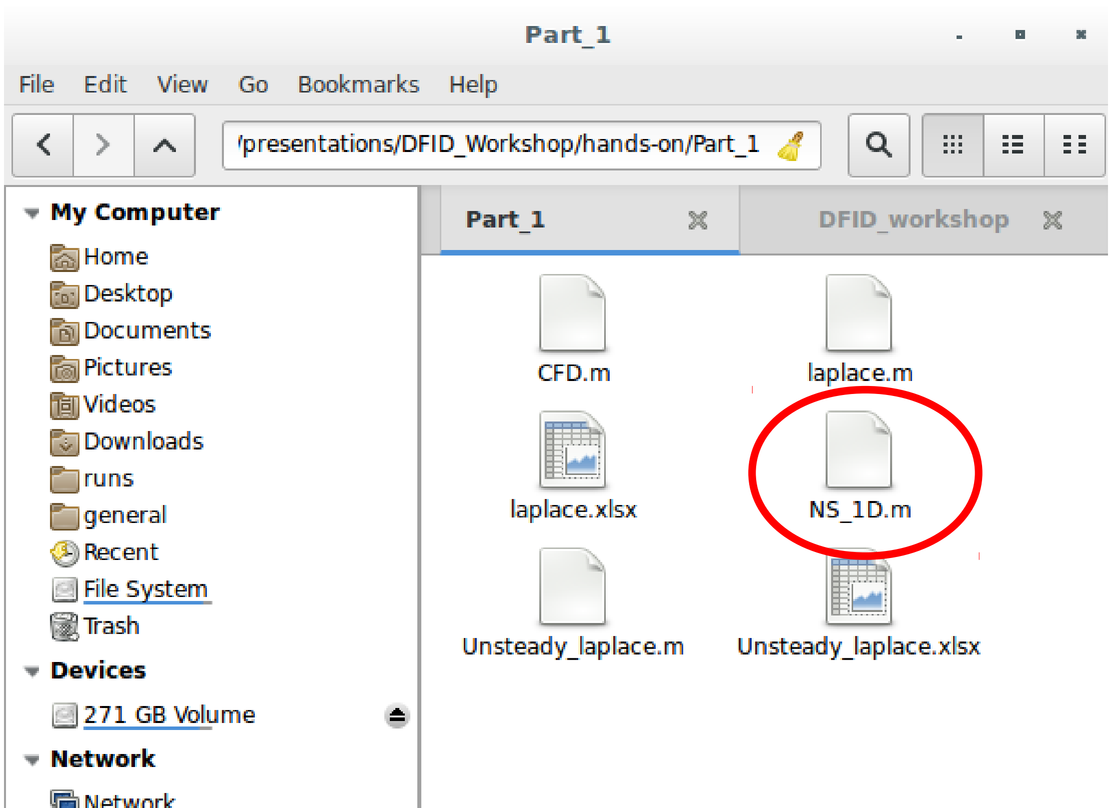
```
clear all
close all
%Setup everything
Lx = 2.0; nx = 44; nt = 300;
dt = 0.0025; nu = 0.1;
dx = Lx/(nx-1.);
u = zeros(nx+1,1); p = zeros(nx,1);
u(10:20) = -1.0;

%iterate through time
for n=1:nt
    %Advection and diffusion
    i = [2:nx]';
    un = u;
    u(i)=u(i)–dt*(un(i).*(un(i+1)...
                               -un(i-1))/(2*dx));
    u(i) = u(i) + dt*nu*(un(i+1) ...
                    -2.0*un(i)+un(i-1))/dx^2;
```

```
   %Solver for Pressure
   for it = 1:100
       pn = p;
       i = [2:nx-2]';
       b = -0.5*(dx)*(u(i+1)-u(i-1));
       p(i) = 0.5*(p(i+1)+p(i-1))+b;
       %Periodic Boundary conditions
       p(1) = p(end-1);  p(end) = p(2);
       if (max(abs(pn-p)) < 1e-4)
           it
           break
       end
   end
   %Apply pressure
   u(i) = u(i) - 2.*dt*(p(i+1)-p(i))/dx;
   %Periodic Boundary conditions
   u(1) = u(end-1);  u(end) = u(2);
end
```

Hands-on Session

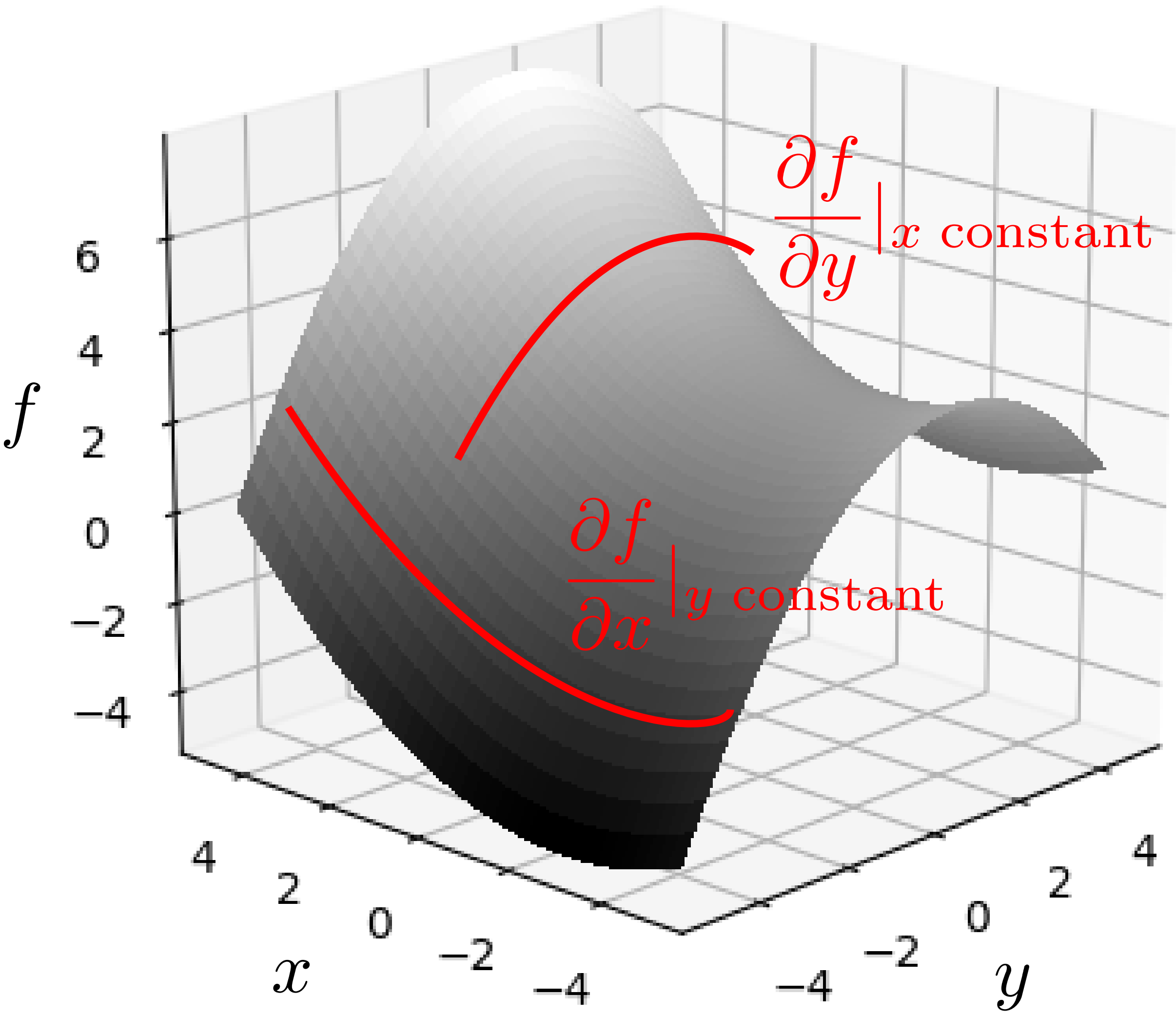
- **1D Navier Stokes Equation**



Slides and hands-on code at

[edwardsmith.co.uk/content/RS-DFID.zip]

Two Dimensions and Partial Derivatives



- Consider a function of two variables

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

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

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

Partial Differential Equations in 2D

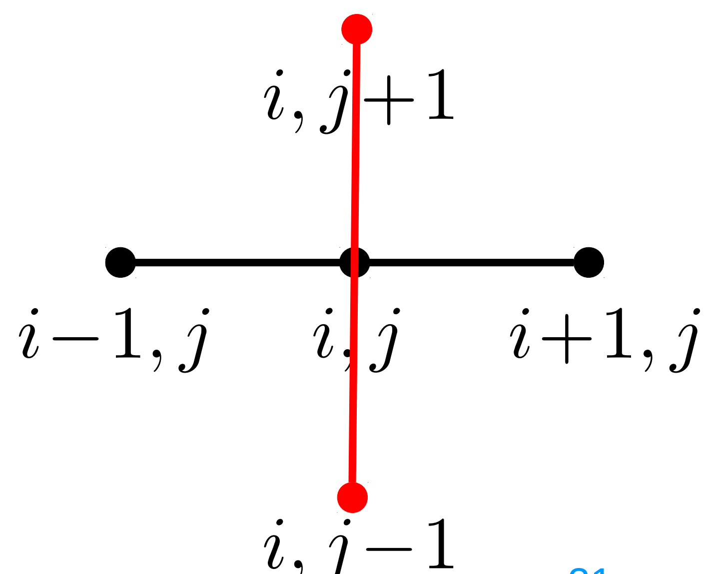
- To describe the change in fields, we use partial differential equations which vary in space (2D here), for example:

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

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

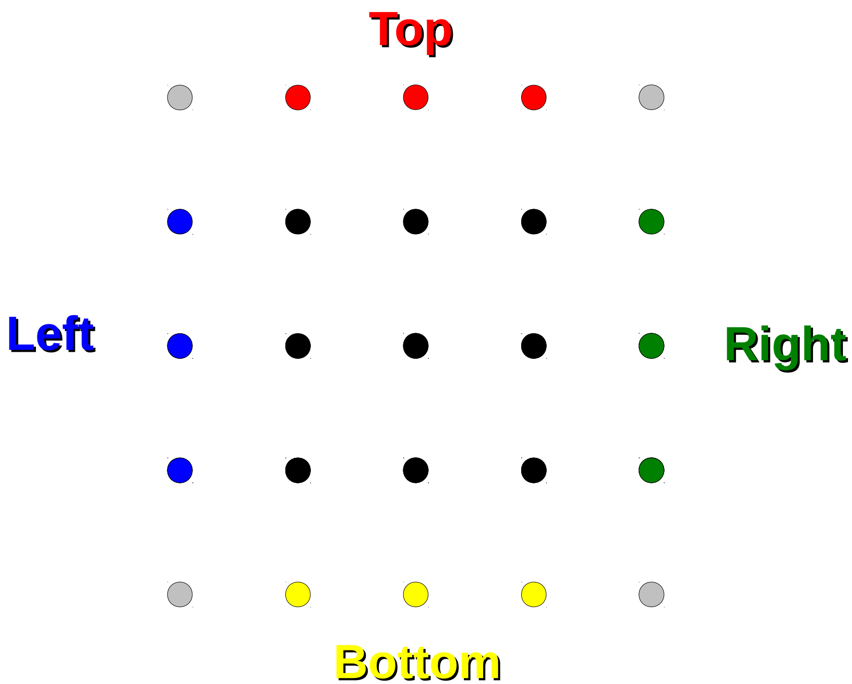
$$\frac{\partial^2 f}{\partial x^2} \approx \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{(\Delta x)^2}$$

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



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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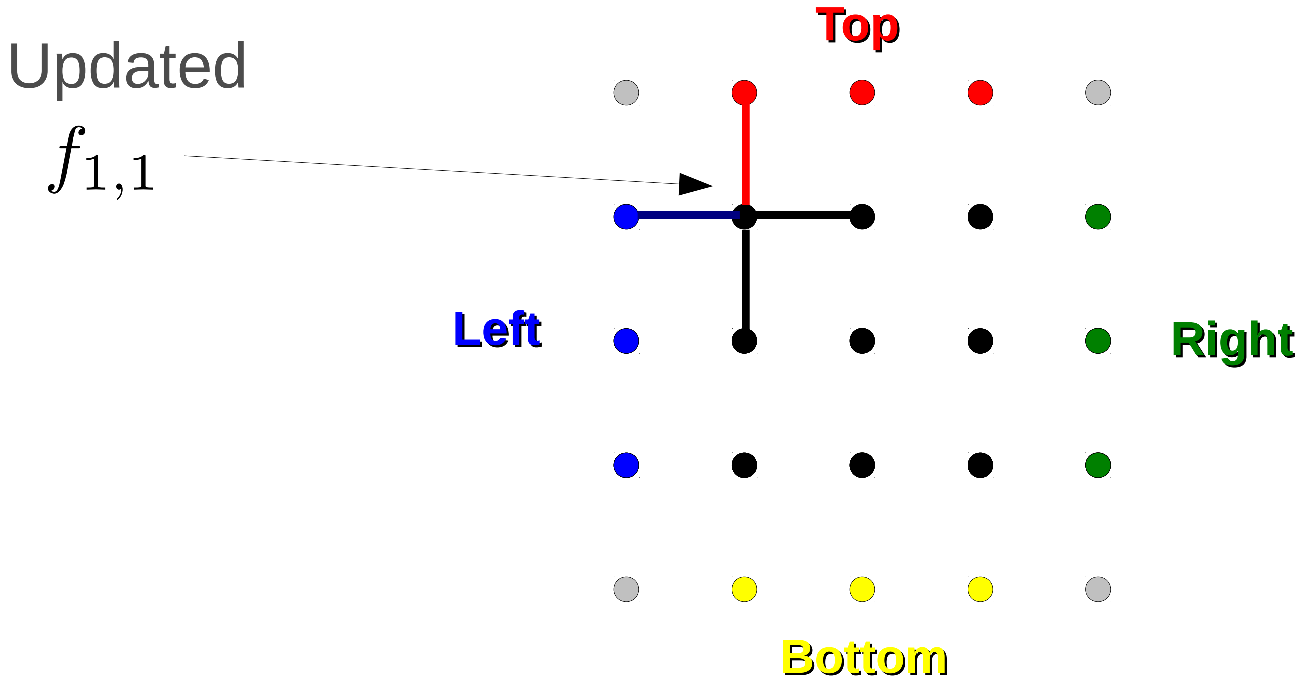

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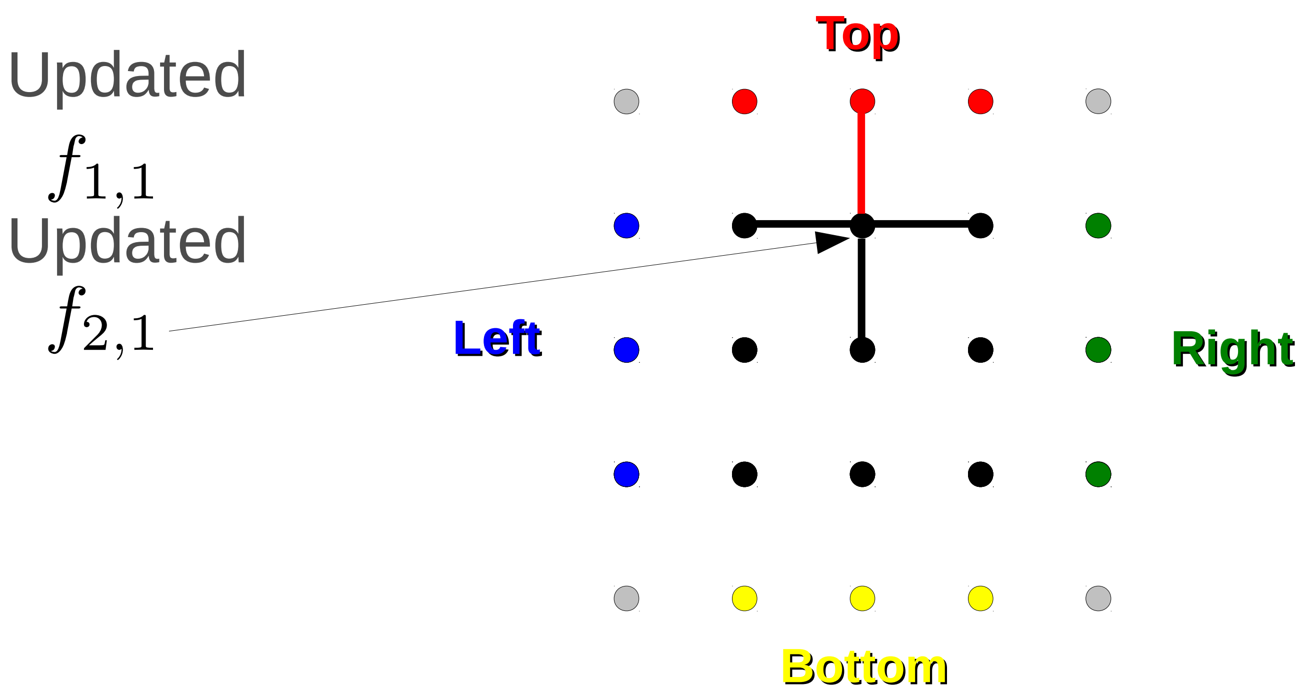


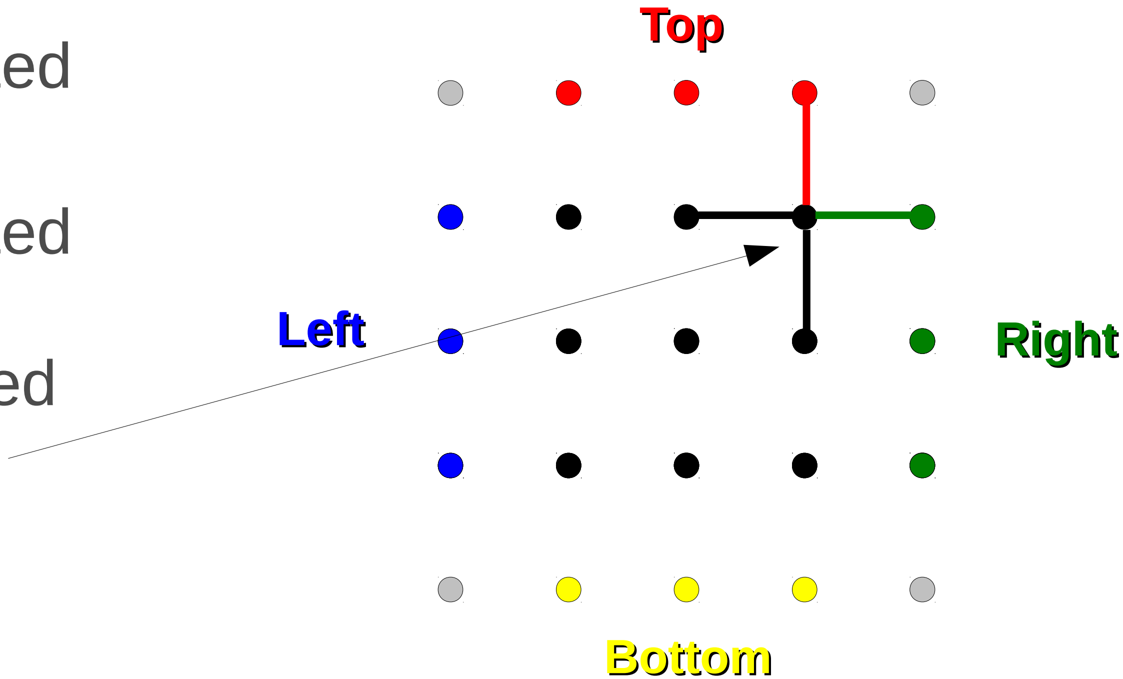
Boundary Conditions

- 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 $f_{3,1}$

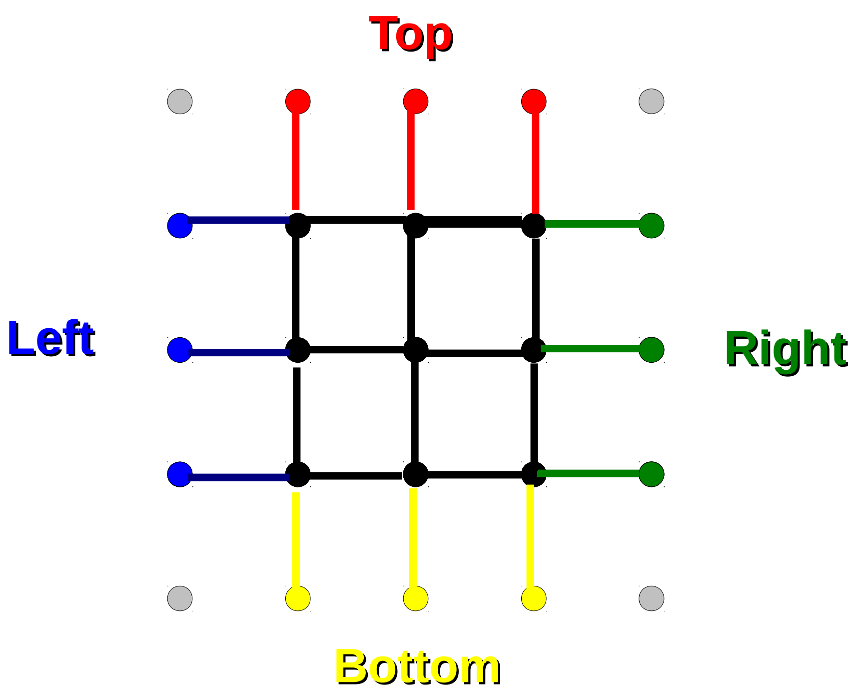


Boundary Conditions

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

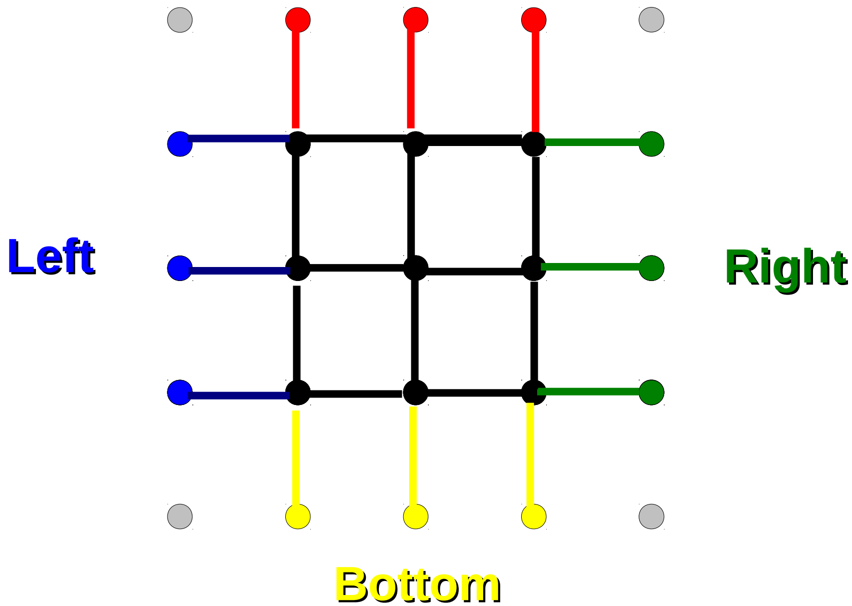
  Updated $f_{1,1}$ $f_{2,1}$ $f_{3,1}$ $f_{1,2}$ $f_{2,2}$ $f_{3,2}$ $f_{1,3}$ $f_{2,3}$ $f_{3,3}$

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

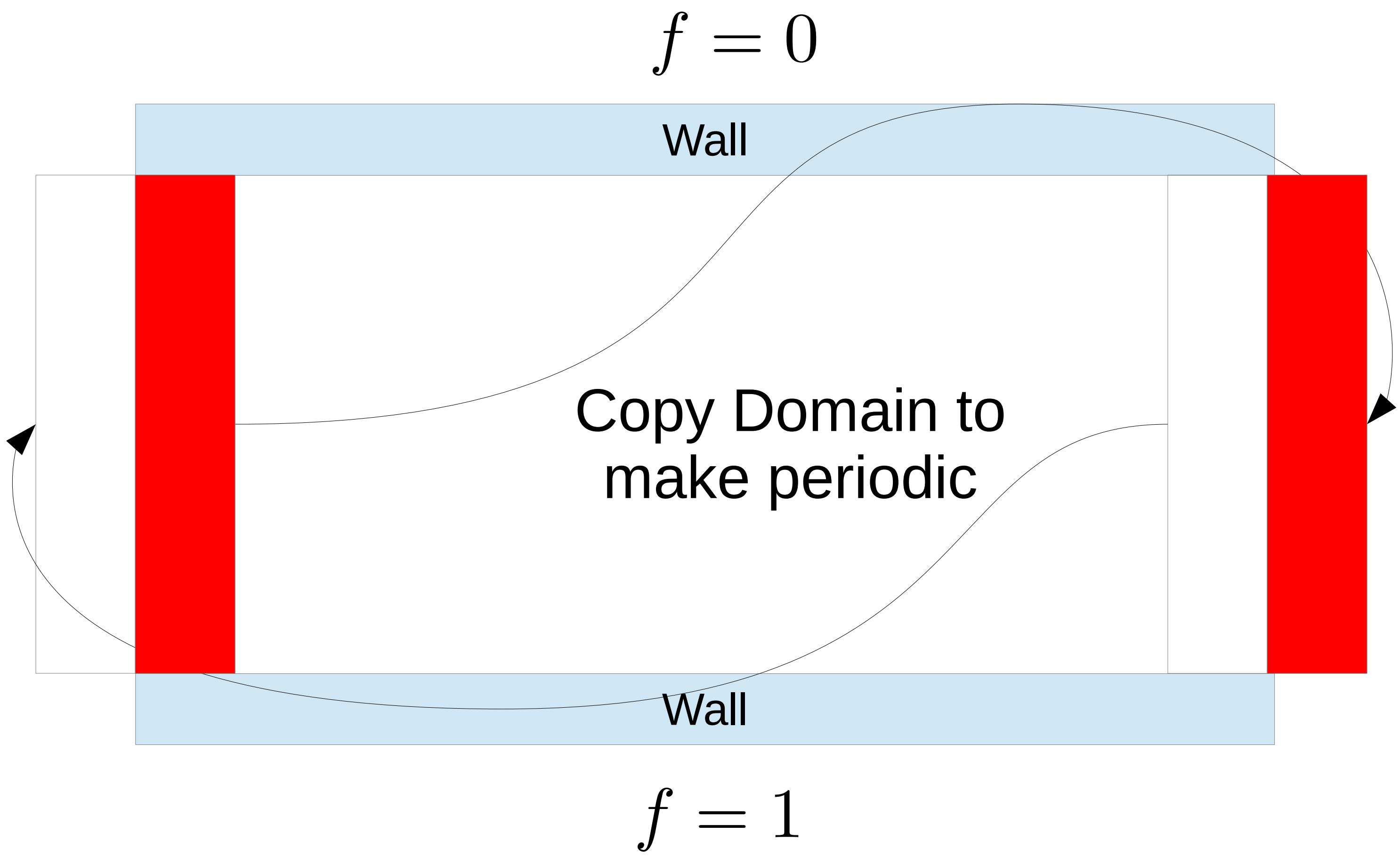


Boundary Conditions

- 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 MATLAB



Boundary Conditions



Partial Differential Equations in 2D

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

C5 =((B5+D5)/$E$14 + (C4+C6)/$E$15)*0.5*$K$14

	A	B	C	D	E	F	G
1		1	1	1	1	1	1
2	0.894	0.89359	0.89352	0.894	0.894	0.893	0.893
3	0.792	0.791529	0.79145	0.791	0.791	0.791	0.791
4	0.694	0.693553	0.69347	0.693	0.693	0.693	0.693
5	0.598	0.598177	0.59306	0.598	0.598	0.598	0.598
6	0.504	0.503451	0.50328	0.503	0.503	0.503	0.504

Hands-on Session

- 1D Navier Stokes Equation
- **Laplace's Equation in 2D**
  - MATLAB – Iterates to convergence
  - Excel (Note iterations are turned on)

Slides and hands-on code at

edwardsmith.co.uk/content/RS-DFID.zip

Functions of Time and Space

- Consider unsteady diffusion

$$\frac{\partial u}{\partial t} = \nu \left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right] \qquad u = u(x, y, t)$$

- We have both a first order time derivative (unsteady term)

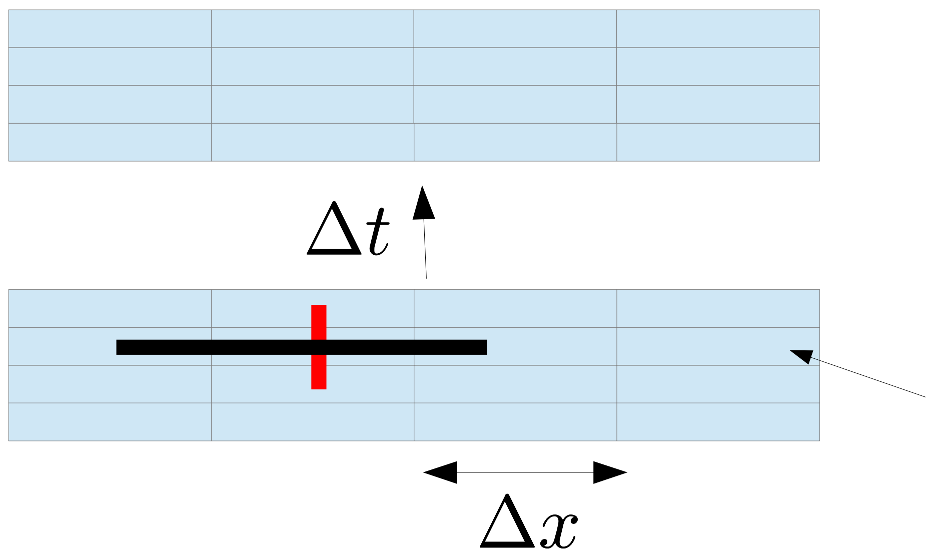
$$\frac{du}{dt} \approx \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} = \frac{u_i^{t+1} - u_i^t}{\Delta t}$$

- and the second order space derivative (diffusion term)

$$\frac{d^2 u}{dx^2} \approx \frac{u_{i+1,j}^t - 2u_{ij}^t + u_{i-1,j}^t}{(\Delta x)^2}, \quad \frac{\partial^2 u}{\partial y^2} \approx \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta y)^2}$$

Functions of Time and Space

- Take each field at time t and calculate the field at the next time



Initial field is important over short times

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

Hands-on Session

- 1D Navier Stokes Equation
- Laplace's Equation in 2D
  - MATLAB – Iterates to convergence
  - Excel (Note iterations are turned on)
- **Unsteady Diffusion Equation in 2D**
  - MATLAB – copies made each loop
  - Excel – A copy for each timestep

Slides and hands-on code at

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Navier Stokes in 2D

- Split time integration into two parts and use mass equation to get pressure

Convection Term

Diffusion Term

Unsteady Term

$$\begin{cases} \dfrac{\boldsymbol{u}_i^* - \boldsymbol{u}_i^t}{\Delta t} = -\boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} - \nu \nabla^2 \boldsymbol{u} \\ \dfrac{1}{\Delta t} \boldsymbol{\nabla} \cdot \boldsymbol{u}_i^* = \dfrac{1}{\rho} \boldsymbol{\nabla}^2 P \end{cases}$$

Pressure Term

Poisson equation - RHS is Laplace's Equation and we need to iterate

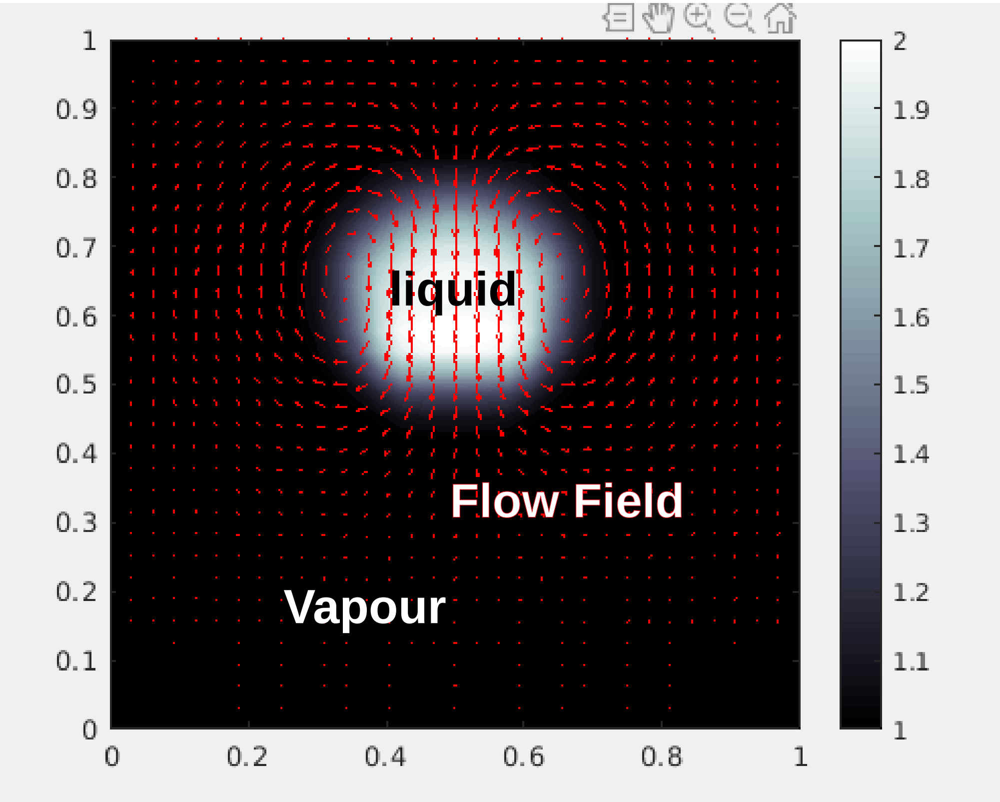
Navier Stokes - Limitations and Extensions

- Only single-phase flows, additional models needed for interface, **nucleation**, contact lines and phase change
- No model for energy, a separate equation if required
- High speed flows (high Mach number) require compressibility to be modelled
- Turbulence requires very large scale simulations or additional models (RANS, LES)
- Flow through porous or granular material more complex
- Non-Newtonian fluid require complex visco-elastic behaviour through additional models

Adding in Multi-Phase Flow

- In order to model boiling, we need to be able to track the location of liquid and vapour regions

- The velocity flow field from the NS equations will then drive the liquid/vapour evolution



- Molecular Dynamics will take care of the nucleation (as we will see in the next section)

* www.nd.edu/~gtryggva/MultiphaseDNS/

Adding in Multi-Phase Flow

- Not a trivial extension, various methods exists, e.g.
  - Volume of Fluid
  - Interface tracking (see later Tryggvason* examples)
  - Levelset
- Here we use the simple approach of Tryggvason*, solve for density propagation to track both liquid/vapour densities

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho u}{\partial x}$$

- With artifical diffusion added for numerical stability reasons

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho u}{\partial x} + \mu_0 \frac{\partial^2 \rho u}{\partial x^2}$$

- Molecular Dynamics will take care of the nucleation (as we will see in the next section)

* www.nd.edu/~gtryggva/MultiphaseDNS/

Adding in Multi-Phase Flow

- Here we use the simple approach of Tryggvason*, solve for density propagation to track both liquid/vapour densities

$$\frac{\partial \rho}{\partial t} = -\frac{\partial \rho u}{\partial x} + \mu_0 \frac{\partial^2 \rho u}{\partial x^2}$$

We evolve the density field in time and use with u* to solve the incompressible pressure field

$$\frac{1}{\Delta t}\boldsymbol{\nabla} \cdot \boldsymbol{u}_i^* = \frac{1}{\rho_i}\boldsymbol{\nabla}^2 P$$

- The boundary conditions for density are set to large values for simplicity, as density appears in denominator of the pressure equation the boundary terms are almost zero

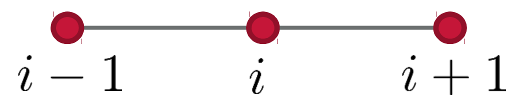
Other Numerical Methods

- The Navier-Stokes Equation

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

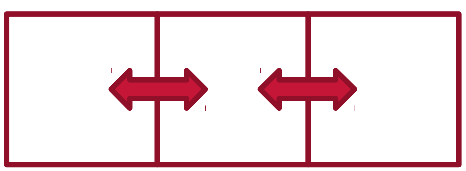
- Finite Difference Method

$$\frac{\partial u_i}{\partial x} \approx \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$



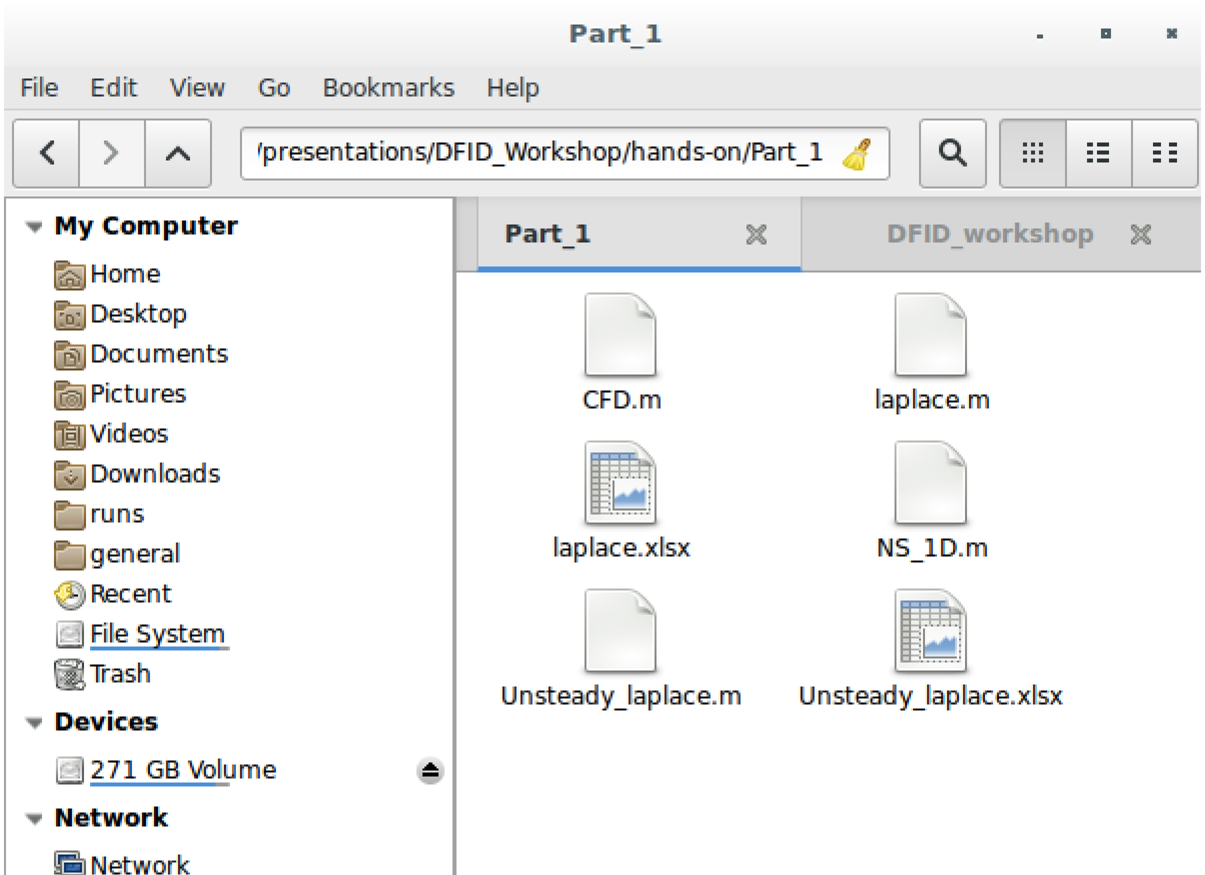
- **Finite Volume Method (used in Tryggvason code)**

$$\frac{\partial}{\partial t}\int_V \rho \boldsymbol{u} dV = -\oint_S \rho \boldsymbol{u}\boldsymbol{u} \cdot d\mathbf{S} - \oint_S \mathbf{\Pi} \cdot d\boldsymbol{S}$$



- Other methods: finite element, spectral methods, smooth particle hydrodynamics, lattice Boltzmann, …

Hands-on Session



Slides and hands-on code at

edwardsmith.co.uk/content/RS-DFID.zip

* www.nd.edu/~gtryggva/MultiphaseDNS/

Brunel University London

Hands-on Session

Slides and hands-on code at **edwardsmith.co.uk/content/RS-DFID.zip**

- 1D Navier Stokes Equation
- Laplace's Equation in 2D
  - MATLAB – Iterates to convergence
  - Excel (Note iterations are turned on)
- Unsteady Diffusion Equation in 2D
  - MATLAB – copies made each loop
  - Excel – A copy for each timestep
- A minimal CFD solver including multi-phase flow
  - Based on minimal code of Tryggvason*
  - See DNS-Solver.pdf file for full details