Numerical Algorithms for HPC

Discretised Partial Differential Equations

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Overview of Lecture

- Pollution problem as a Partial Differential Equation (PDE)
  - equations in one and two dimensions
  - boundary conditions
- Discretised equations
  - putting problem onto a lattice
  - PDE as a matrix problem
  - the five-point stencil
  - mapping between the 2D continuous and discrete problems
  - introducing a wind into pollution problem
- Notes
- Summary

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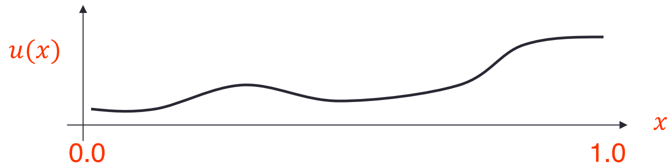
1D Diffusion Equation

- Imagine one-dimensional problem *with no wind*
  - e.g. pollution in a valley
- Call the density of pollution u
  - distance along the valley is x which is in the range $[0.0, 1.0]$
    - in general the domain size is L, but for simplicity we take $L = 1.0$



- Differential equation is: $-\frac{d^2}{dx^2}u(x) = 0$
  - initial minus sign is a useful convention (see later)
  - equation is for steady state solution that does not vary in time

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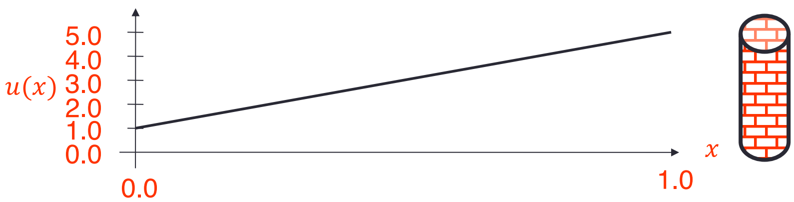
Analytic Solution

- In one dimension, solution is a straight line
  - equation is: $u(x) = m\,x + c$
  - but what are the values of gradient m and intercept c?
- Actual solution depends on *boundary conditions*
  - differential equation gives the behaviour in the interior (0.0,1.0)
  - must also specify the behaviour at boundaries $x = 0.0$ and $x = 1.0$
  - for example, $u(0.0) = 1.0$ and $u(1.0) = 5.0$



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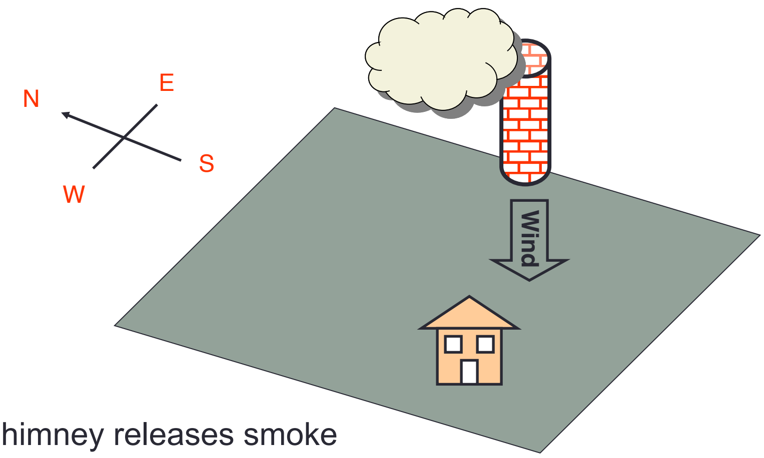
Boundary Conditions

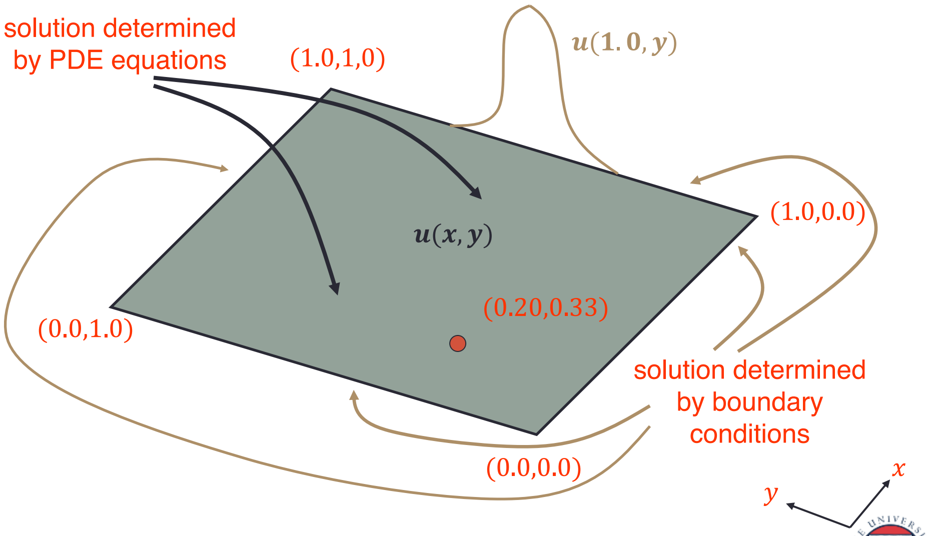
- We solved the equation: $-\frac{d^2}{dx^2}u(x) = 0$
  - with $u(0.0) = 1.0$ and $u(1.0) = 5.0$, the answer is $u(x) = 4.0\,x + 1.0$
- In general
  - "What is the pollution in a valley?" is a meaningless question
  - must ask: "What is the pollution in a valley when the pollution levels are **one** at the western end and **five** at the eastern end?"
- Same applies in the 2D problem
  - equations will determine solution $u(x, y)$ in the **interior** region
  - we must independently specify behaviour on all the **boundaries**
- For this reason, steady state problems like this are called *Boundary Value Problems (BVPs)*

The Problem we want to solve



- Chimney releases smoke
  - how much arrives at house with prevailing north-easterly wind?

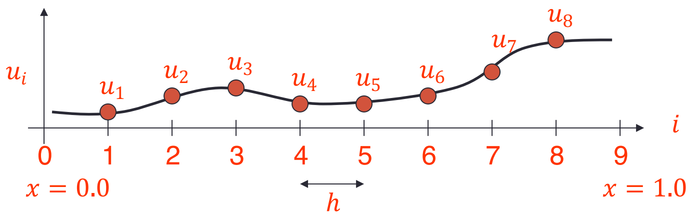
Use 2D Domain (x, y) of Size 1×1



Mathematical Problem in 2D

- PDE with no wind is $-\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) u(x, y) = 0$
  - all solutions obey this Partial Differential Equation (PDE) in interior region
- Must also specify Boundary Conditions (BCs)
  - BCs must be **appropriate to our specific problem**
- In this case, a simple choice is:
  - set pollution on boundary to zero **everywhere** except at chimney
    - assume domain is large enough that no pollution gets to the edges
  - specify $u(1.0, y)$ as a hump concentrated around $(1.0, 0.5)$
    - this is a guess at the way pollution is emitted by the chimney
    - a single sharp peak at $(1.0,0.5)$ causes technical problems later!
- Solve the equations somehow ...
  - and the pollution level at the house is the value of $u(0.20,0.33)$

Discretising the 1D Problem



- Replace continuous real x by discrete integer i
  - divide domain into a lattice containing $M + 1$ sections each of width h
  - e.g. in above diagram, $M = 8$ and $h = 1.0/(M + 1) = 0.11$
- Solve for N different variables $u_i, \quad i = 1, 2, \ldots, N$
  - in one dimension, $N = M$ but not true in general (in 2D problem $N = M^2$)
  - boundary values are u_0 and u_{N+1} (above, u_0 and u_9)
- But what equations do the u_i variables satisfy?
  - and how do we decide on the boundary values?

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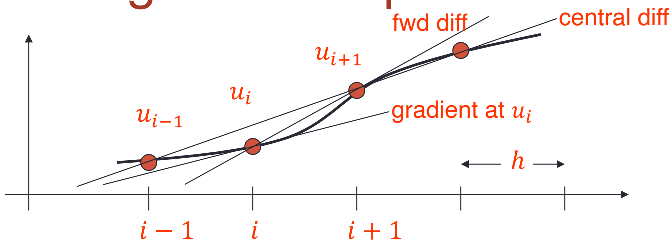
Discretising the 1D Equations



- We approximate gradients with lines
  - e.g. a forward difference: $\frac{d}{dx}u(x) \approx \frac{u_{i+1}-u_i}{h}$
  - or a central difference: $\frac{d}{dx}u(x) \approx \frac{u_{i+1}-u_{i-1}}{2h}$
- All become more accurate as we reduce h
  - but for a given value of h, some will be more accurate than others
  - e.g. forward difference has errors proportional to h
    - central has errors proportional to h^2 and is therefore **more accurate**
  - can estimate errors by doing a Taylor expansion about $u(x)$ ...

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Discretised 1D Equations

- Write second derivative as: $\frac{d^2}{dx^2}u(x) = \frac{d}{dx}\left(\frac{d}{dx}u(x)\right)$
  - use forward difference for first derivative, then a backward for second

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

- Boundary conditions are straightforward

$$u(0.0) = 1.0: \quad u_0 = 1.0$$
$$u(1.0) = 5.0: \quad u_{M+1} = 5.0$$

- This gives us N equations in N unknowns

$$-u_{i-1} + 2u_i - u_{i+1} = 0, \quad i = 1, 2, \ldots, N$$

- Converted differential equations into difference equations
  - larger M means a smaller h and more accurate equations
  - but also a larger N and much more work, especially in 2D or 3D problems!

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Difference Equations for $N = 8$

- Writing the eight equations $-u_{i-1} + 2u_i - u_{i+1} = 0$ out in full

$$\begin{aligned}
2u_1 - u_2 &= 1 \\
-u_1 + 2u_2 - u_3 &= 0 \\
-u_2 + 2u_3 - u_4 &= 0 \\
-u_3 + 2u_4 - u_5 &= 0 \\
-u_4 + 2u_5 - u_6 &= 0 \\
-u_5 + 2u_6 - u_7 &= 0 \\
-u_6 + 2u_7 - u_8 &= 0 \\
-u_7 + 2u_8 &= 5
\end{aligned}$$

- Notes
  - have multiplied all the equations by h^2 for simplicity
  - first and last equations are different as we know u_0 and u_9
  - we write the known values on the right-hand-side for convenience

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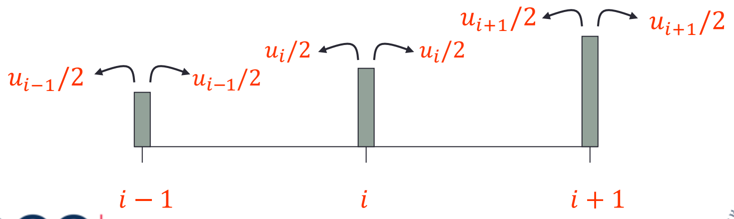
Interpreting Difference Equations

- Simple interpretation
  - Rearranging gives $u_i = (u_{i+1} + u_{i-1})/2$
  - i.e. every point equals the average of its nearest neighbours
  - what has this got to do with diffusion?
- Imagine pollution particles do "a random walk"
  - each step, particles at every lattice point move randomly left or right
  - let u_i be the number of particles at lattice point i



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Steady State Random Walk

- At each step
  - population u_i is replaced by $u_{i-1}/2$ (from left) and $u_{i+1}/2$ (right)
  - for a steady state, $u_i = (u_{i-1} + u_{i+1})/2$
  - same equations as before: $-u_{i-1} + 2u_i - u_{i+1} = 0,\ i = 1,2,\ldots,N$
- Perhaps easier to understand than: $-\dfrac{d^2}{dx^2}u(x) = 0$
- Note that this is a dynamic equilibrium
  - just because pollution level $u(x)$ is constant doesn't mean that the pollution particles are static
  - e.g. density of air is constant even though molecules are moving!

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Equations in Matrix Form

- These can be written in standard form $Au = b$

$$\begin{pmatrix} 2 & -1 & & & & & & \\ -1 & 2 & -1 & & & & & \\ & -1 & 2 & -1 & & & & \\ & & -1 & 2 & -1 & & & \\ & & & -1 & 2 & -1 & & \\ & & & & -1 & 2 & -1 & \\ & & & & & -1 & 2 & -1 \\ & & & & & & -1 & 2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 5 \end{pmatrix}$$

  - in this case, A is sparse and symmetric

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Two Dimensional Problem

- Simple extension to two dimensions
  - impose a square lattice of size $M+1$ by $M+1$, spacing h
  - replace real continuous coordinates (x, y) by integers i, j
  - solution is now $u_{i,j}$ with $i = 1, 2, \dots, M$ and $j = 1, 2, \dots, M$
  - the number of unknowns N is now M^2

  - in 1D: $\frac{d^2}{dx^2}u(x) \approx \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2}$

  - in 2D: $\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)u(x, y) \approx \frac{u_{i,j-1} + u_{i-1,j} - 4u_{i,j} + u_{i+1,j} + u_{i,j+1}}{h^2}$

  - every point is averaged with its **four nearest neighbours**

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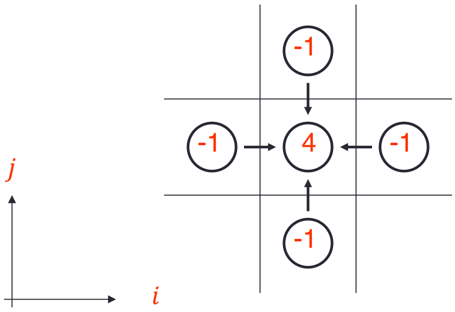
Five Point Stencil

- The equation can be represented graphically
  - (remember the initial minus sign!)
  - again, can easily be interpreted as a random walk



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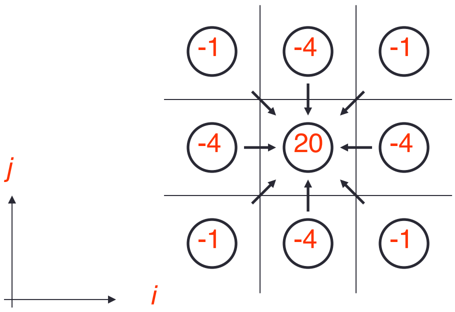
More Accurate Stencils

- More accuracy means more complicated shape
  - e.g. a nine-point stencil for the same equation includes $u_{i+1,j+1}$, …
  - can be understood as a random walk, now also including diagonals



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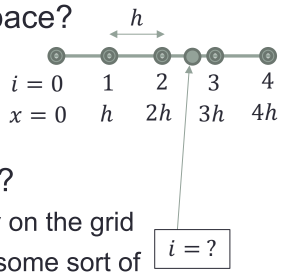
Notation

- The vector b is often called the *source*
  - remember that it contains all the fixed boundary values of u
  - for 2D problem, corresponds to hump function around chimney
    - the hump is clearly the *source* of the pollution
- The 2D diffusion operator is very common
  - has a special name, “Grad Squared”, and symbol: ∇^2
- Can write the 2D equations as: $-\nabla^2 u(x,y) \;=\; 0$
  - the five-point stencil is a standard discretisation of ∇^2
  - different discretisations (or different equations) will lead to a different form for the matrix *A*
- Another notation indicates derivatives by a dash: u'

$$\frac{d}{dx}u(x) \longrightarrow u'(x), \qquad \frac{d^2}{dx^2}u(x) \longrightarrow u''(x)$$

Grid Coordinates vs Real Space

- We store values on a discrete grid
  - $u_0, u_1, u_2, \ldots, u_{N-1}, u_N, u_{N+1}$
- What points do these represent in real space?
  - in 1D: $x \;=\; ih$ $\qquad u_i \;\rightarrow\; u(ih)$
  - in 2D: $x \;=\; ih, y \;=\; jh$ $\qquad u_{i,j} \;\rightarrow\; u(ih, jh)$



- Converting from real space to grid points?
  - much harder as coordinate x will not sit exactly on the grid
  - to get the value of $u(x)$ from the grid, must do some sort of interpolation of u_i from the nearby grid points
  - simplest solution is a weighted average – see exercise notes

Introducing a Wind

- More pollution moves in same direction as wind
  - in 1D, the equations for a wind of strength a (from the right) are

$$-\frac{d^2}{dx^2}u(x) - a\frac{d}{dx}u(x) = 0$$

$$\frac{-u_{i-1}+2u_i-u_{i+1}}{h^2} - a\left(\frac{u_{i+1}-u_i}{h}\right) = 0$$

$$-\left(\frac{1}{h^2}\right)u_{i-1} + \left(\frac{2}{h^2}-\frac{a}{h}\right)u_i - \left(\frac{1}{h^2}+\frac{a}{h}\right)u_{i+1} = 0$$

  - more particles move left (from u_{i+1} to u_i) than right
    - makes the associated matrix A non-symmetric
    - straightforward to extend to two dimensions

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In Two Dimensions

- 2D equations for a NE wind of strength (a_x, a_y)

$$-\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)u(x,y) - a_x\frac{\partial}{\partial x}u(x,y) - a_y\frac{\partial}{\partial y}u(x,y) = 0$$

- Use forward differences for first derivatives, e.g.:

$$\frac{\partial}{\partial x}u(x,y) \approx \frac{u_{i+1,j}-u_{i,j}}{h}$$

  - now straightforward to write out difference equations in full
  - on the computer we deal with the values $a_x h$ and $a_y h$

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Notes

- What about different boundary conditions?
  - fixed boundary conditions are called Dirichlet conditions
  - might want to specify the gradient at a boundary
    - e.g. "the slope of the pollution curve should be zero at the edges"
    - these are called Neumann boundary conditions
- Dirichlet conditions affect the right-hand-side b
  - Neumann conditions alter the matrix A near domain boundaries
- Non-Linear Equations
  - can easily be discretised using standard recipes
  - this will lead to equations like: $u_1^2 + 2\,u_2 + u_3 = 0$
  - this CANNOT be expressed as a matrix equation with constant A
    - i.e. not possible to solve using methods like Gaussian Elimination

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Summary

- Many physical problems are expressed as PDEs
  - impose a regular lattice on the problem
  - discretise the differential equations using standard techniques
- This leads to set of N difference equations
  - converts PDE to a set of linear equations $Au = b$ which we can solve
  - A depends on the PDE, b on boundary conditions, solution is u
  - N may be very large indeed for 2D or 3D problems!
- We are solving an approximation to the PDE
  - even if we solve linear equations accurately, there is still an error
  - can reduce this error using a more accurate discretisation of PDE
    - or a larger M (i.e. smaller value of h) with the same discretisation
  - both these approaches require additional work

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