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Parallel Numerical Algorithms

Discretised Partial Differential Equations

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▶ Pollution problem as a Partial Differential Equation
  – 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

▶ Notes

▶ Summary

► Imagine one-dimensional problem *with no wind*
  – eg 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

u(x)

0.0   1.0   *x*
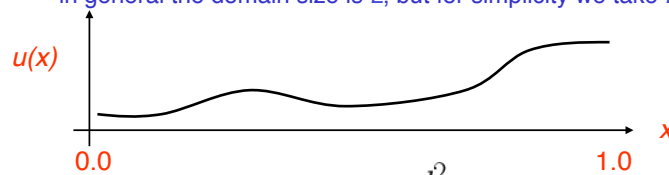
► Differential equation is: $-\dfrac{d^2}{dx^2}\,u(x) = 0$

  – 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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► 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

5.0
4.0
u(x) 3.0
2.0
1.0
0.0

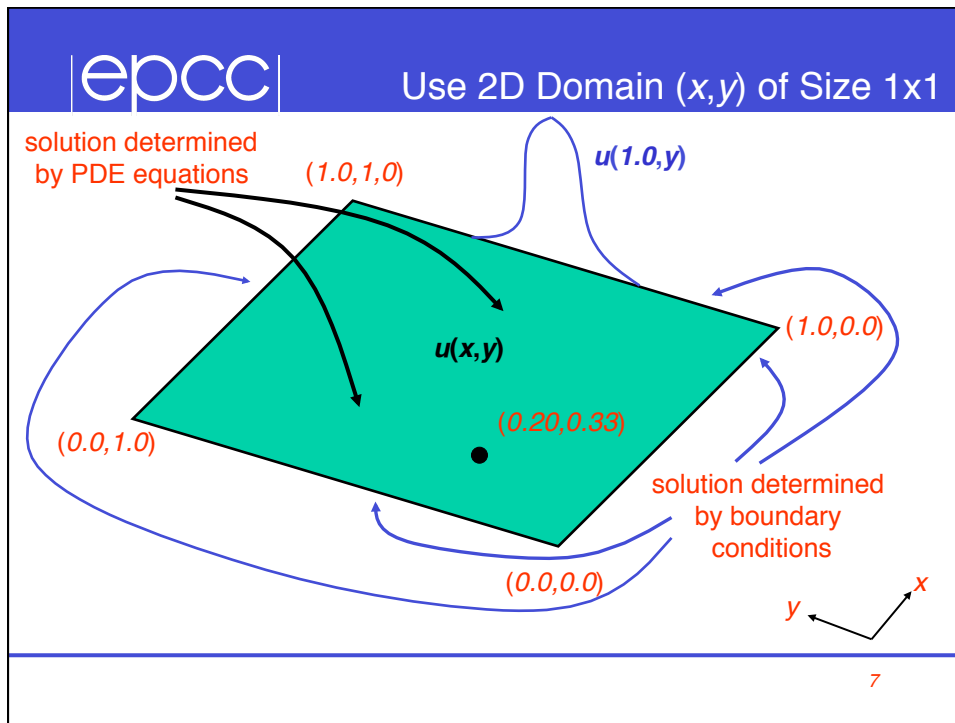0.0   1.0   *x*

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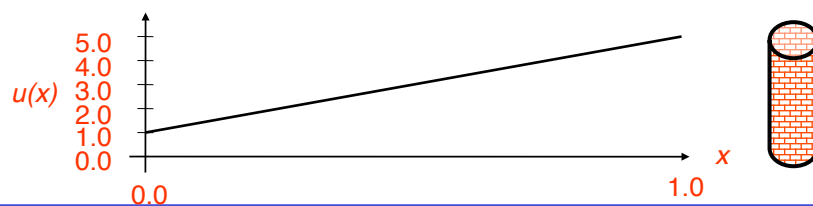
- We solved the equation: $-\dfrac{d^2}{dx^2}u(x) = 0$

  - 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 our two-dimensional 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*

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The Problem we want to solve
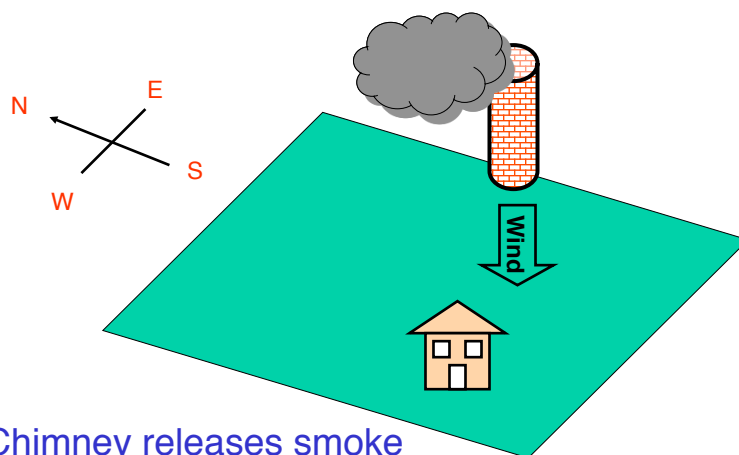
- Chimney releases smoke
  - how much arrives at house with prevailing north-easterly wind?

solution determined
by PDE equations
(*1.0,1,0*)

u(1.0,y)

u(x,y)

(*1.0,0.0*)

(*0.20,0.33*)

(*0.0,1.0*)

solution determined
by boundary
conditions

(*0.0,0.0*)

x

y

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▸ 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 $u(0.20,0.33)$

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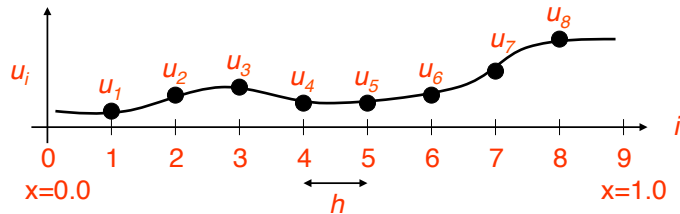
- Replace continuous real *x* by discrete integer *i*
  - divide domain into a lattice containing *M*+1 sections each of width *h*
  - eg in above diagram, *M*=8 and *h* = 1.0/(*M*+1) = 0.11
- Solve for *N* different variables u_i, *i* = 1, 2, ... *N*
  - in one dimension, *N* = *M* but not true in general (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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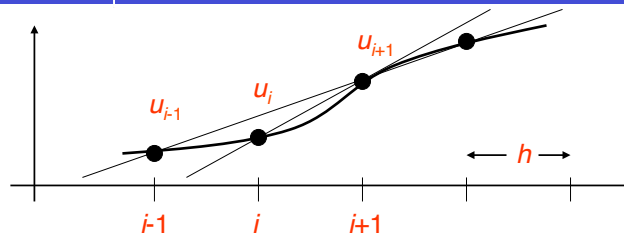
- Approximate gradients with lines,
  - eg a forward difference:

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

  - 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
  - eg 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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▸ Write second derivative as: $\dfrac{d^2}{dx^2}\,u(x) = \dfrac{d}{dx}\left(\dfrac{d}{dx}\,u(x)\right)$

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

▸ This gives us N equations in N unknowns
  - $u_{i-1} + 2\,u_i - u_{i+1} = 0$, $i = 1, 2, \dots N$

▸ 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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▸ Writing the eight equations 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
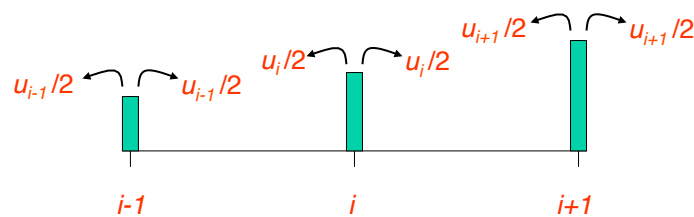
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▶ Simple interpretation
– every point equals the average of its nearest neighbours
– what has this got to do with diffusion?

▶ 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

$u_{i-1}/2$ ⟶ ⟶ $u_{i-1}/2$ $u_i/2$ ⟶ ⟶ $u_i/2$ $u_{i+1}/2$ ⟶ ⟶ $u_{i+1}/2$

i-1   *i*   *i+1*

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

▶ 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
– eg density of air is constant even though molecules are moving!

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‣ These can be written in standard form *Au = b*

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

– in this case, *A* is sparse and symmetric

‣ 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, ... *M* and *j* = 1, 2, ... *M*
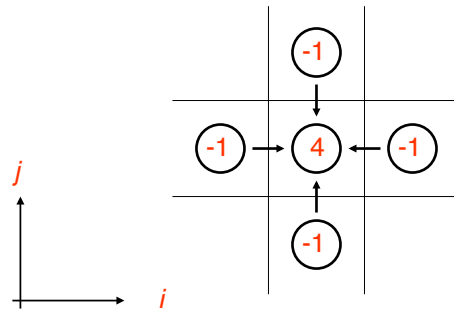   – the number of unknowns *N* is now M^2

   – in 1D $\qquad \dfrac{d^2}{dx^2}\, u(x) \approx \dfrac{u_{i-1} - 2u_i + u_{i+1}}{h^2}$

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

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

Five Point Stencil

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

More Accurate Stencils

▶ More accuracy means more complicated shape
   – eg 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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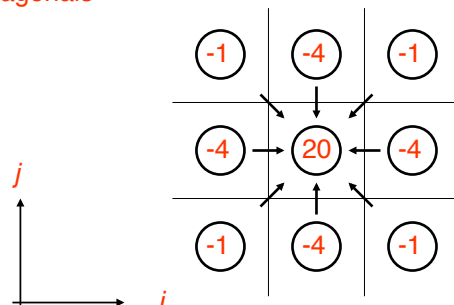
▸ The vector *b* is often called the *source*
  – remember that it contains all the fixed boundary values of *u*
  – for 2D problem, corresponds to hump function around chimney
    • the hump is clearly the *source* of the pollution
▸ The 2D diffusion operator is very common
  – has a special name, "Grad 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 '

$$\frac{d}{dx}\,u(x) \rightarrow u'(x), \quad \frac{d^2}{dx^2}\,u(x) \rightarrow u''(x)$$

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▸ We store values on a discrete grid
  – $u_0, u_1, u_2, \dots, u_{N-1}, u_{N+1}$

▸ What points do these represent in real space?
  – in 1D: $x = i{*}h$ $u_i \rightarrow u(i{*}h)$
  – in 2D: $x = i{*}h$, $y = j{*}h$ $u_{i,j} \rightarrow u(i{*}h, j{*}h)$

▸ 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

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▶ 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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▶ 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, eg:

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

  – 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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▸ What about different boundary conditions?
- fixed boundary conditions are called Dirichlet conditions
- might want to specify the gradient at a boundary
  - eg "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*
  - ie not possible to solve using methods like Gaussian Elimination

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▸ 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* (ie smaller value of *h*) with the same discretisation
- both these approaches require additional work

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