

# PDE and Boundary-Value Problems

## Winter Term 2015/2016

### Lecture 21

Saarland University

5. Februar 2016

## Purpose of Lesson

- To introduce the idea of explicit finite-difference methods and show how they can be used to solve hyperbolic and parabolic problems.
- To show how time-dependent problems can be solved by another finite-difference scheme known as **implicit methods**.

- We can solve elliptic BVPs (steady-state problems) where the PDE was satisfied in a given region of space, and the solution (or its derivative) was specified on the boundary.
- In those types of problems, we find the approximate solution at the **interior grid points** by solving a system of algebraic equations. In other words, the solution at all the interior grid points was found **simultaneously**.

- To explain the basic philosophy of Monte Carlo methods and suggest how they can be used to solve various problems.
- To show how random games (Monte Carlo methods) can be designed whose outcomes approximate solutions to differential equations. A specific game (tour du wino) is described whose outcome is the finite-difference approximation to a Dirichlet problem inside a square. The game is extended to include solutions to other problems as well.

# An Explicit Finite-Difference Method

- Now we will show how **time-dependent problems** can be solved by finite-difference approximations.
- The idea is that if we are given the solution when time is **zero**, we can then find the solution for  $t = \Delta t, 2\Delta t, 3\Delta t, \dots$  by means of a **marching process**.
- Replacing both the **space** and **time** derivatives by their finite-difference approximations, we can then solve for the solution  $u_{i,j}$  in the difference equation **explicitly** in terms of the solution at earlier values of time.
- This process is called an **explicit-type marching process**, since we find the solution at a **single** value of time in terms of the solution at earlier values of time.

# The Explicit Method for Parabolic Equations

- To show how the explicit finite-difference method works, we consider a representative problem from heat flow.
- Heat flows along a rod initially at temperature zero, where the left end of the rod is fixed at temperature one, and the right-hand side experiences a heat loss (or gain) proportional to the difference between the temperature at that end and an outside temperature that is given by  $g(t)$ .

# The Explicit Method for Parabolic Equations (cont.)

## Problem 21-1

To find a function  $u(x, t)$  that satisfies

$$\text{PDE: } u_t = u_{xx}, \quad 0 < x < 1, \quad 0 < t < \infty$$

$$\text{BCs: } \begin{cases} u(0, t) = 1 \\ u_x(1, t) = -[u(1, t) - g(t)] \end{cases} \quad 0 < t < \infty$$

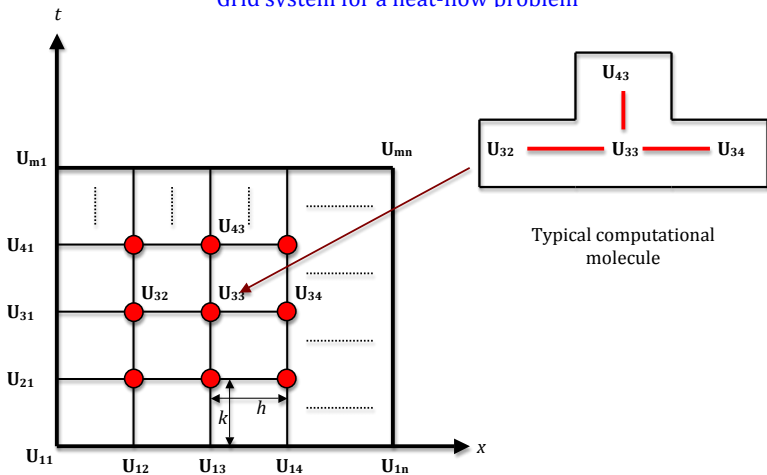
$$\text{IC: } u(x, 0) = 0 \quad 0 \leq x \leq 1$$

To solve problem 21-1 by finite differences, we start by drawing the usual rectangular grid system with grid points

$$x_j = jh \quad j = 0, 1, 2, \dots, n$$

$$t_i = ik \quad i = 0, 1, 2, \dots, m$$

## Grid system for a heat-flow problem





- Note that on the figure of the grid system, the  $u_{i,j}$  on the **left** and **bottom** are given BCs and ICs, and our job is to find the other  $u_{i,j}$ 's.
- To do this, we begin by replacing the partial derivatives  $u_t$  and  $u_{xx}$  in the heat equation with their approximations

$$u_t = \frac{1}{k} [u(x, t + k) - u(x, t)] = \frac{1}{k} (u_{i+1,j} - u_{i,j})$$
$$u_{xx} = \frac{1}{h^2} [u(x + h, t) - 2u(x, t) + u(x - h, t)]$$
$$= \frac{1}{h^2} (u_{i,j+1} - 2u_{i,j} + u_{i,j-1})$$

- By substituting these approximations into  $u_t = u_{xx}$  and solving for the solution at the largest value of time, we have

$$u_{i+1,j} = u_{i,j} + \frac{k}{h^2} [u_{i,j+1} - 2u_{i,j} + u_{i,j-1}] \quad (21.1)$$

### Remark

(21.1) is the formula we are looking for, since it gives us the solution at one value of time in terms of the solution at earlier values of time.

- We are almost ready to begin the computations for problem 21-1. First, we must approximate the derivatives in the right-hand BC

$$u_x(1, t) = - [u(1, t) - g(t)]$$

by

$$\frac{1}{h} [u_{i,n} - u_{i,n-1}] = - [u_{i,n} - g_i], \quad (21.2)$$

where  $g_i = g(ik)$  is given.

- Note that in (21.2) we have replaced  $u_x(1, t)$  by the **backward-difference approximation**, since the forward-difference approximation would require knowing values of  $u_{i,j}$  outside the domain.
- Solving (21.2) for  $u_{i,n}$  gives us

$$u_{i,n} = \frac{u_{i,n-1} + hg_i}{1 + h}. \quad (21.3)$$

# Algorithm for the Explicit Method

1. Find the solution at the grid points for  $t = \Delta t$  by using the explicit formula

$$u_{2,j} = u_{1,j} + \frac{k}{h^2} [u_{1,j+1} - 2u_{1,j} + u_{1,j-1}] \quad j = 2, 3, \dots, n-1$$

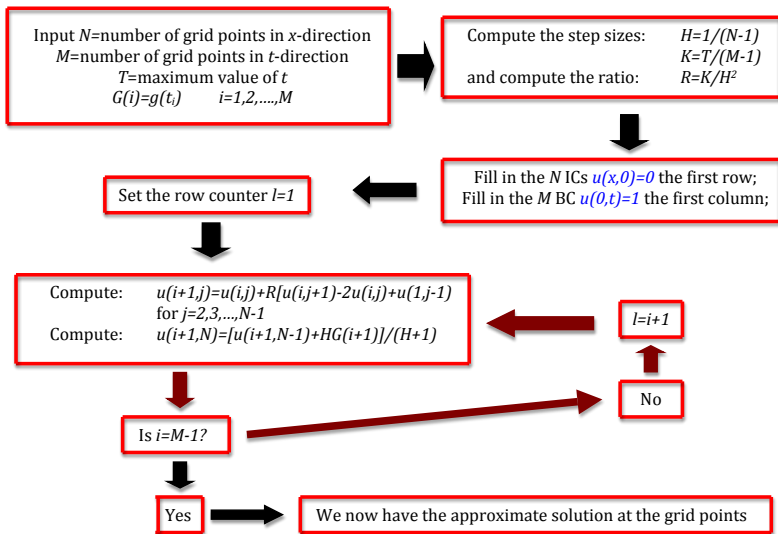
2. Find  $u_{2,n}$  from formula (21.3)

$$u_{2,n} = \frac{u_{2,n-1} + hg_2}{1 + h}.$$

## Remark

- Steps 1 and 2 find the solution for  $t = \Delta t$ .
- To find the solution for  $t = 2\Delta t$  repeat steps 1 and 2, moving up one more row (increase  $i$  by 1) and using the values of  $u_{i,j}$  just computed.
- For  $t = 3\Delta t, 4\Delta t, \dots$  keep repeating the same process.

On the flow diagram on the next page we explain in a precise manner how the computations should be carried out.



## Remarks

- There is a serious deficiency in the explicit method, for if the step size in  $t$  is large compared to the step size in  $x$ , then machine roundoff error can grow until it ruins the accuracy of the solution.
- The relative size of these steps depends on the particular equation and the BCs, but, generally, the step size in  $t$  should be much smaller than the step size in  $x$ . We must have  $k/h^2 \leq 0.5$  in order this method to work.
- A general rule of thumb is that as the step sizes  $\Delta t$  and  $\Delta x$  are made smaller, the **truncation error** of approximating partial derivatives by finite differences decreases. However, the smaller these grid sizes, the more computations necessary, and, hence, the **roundoff error**, as a result of rounding off our computations, will increase.

# The Explicit Method for Hyperbolic Equation

## Problem 21-2

To find a function  $u(x, t)$  that satisfies

$$\text{PDE: } u_{tt} = u_{xx}, \quad 0 < x < 1, \quad 0 < t < \infty$$

$$\text{BCs: } \begin{cases} u(0, t) = g_1(t) \\ u(1, t) = g_2(t) \end{cases} \quad 0 < t < \infty$$

$$\text{ICs: } \begin{cases} u(x, 0) = \phi(x) \\ u_t(x, 0) = \psi(x) \end{cases} \quad 0 \leq x \leq 1$$



- Problem 21-2 can also be solved by the explicit finite-difference method. Here, we can approximate the derivatives  $u_{tt}$  and  $u_{xx}$  by

$$u_{tt} \cong \frac{1}{k^2} [u(x, t + k) - 2u(x, t) + u(x, t - k)]$$
$$u_{xx} \cong \frac{1}{h^2} [u(x + h, t) - 2u(x, t) + u(x - h, t)]$$

and the derivative  $u_t(x, 0)$  in the IC by

$$u_t(x, 0) \cong \frac{1}{k} [u(x, k) - u(x, 0)] = \frac{1}{k} [u(x, k) - \phi(x)].$$

- Solving for  $u(x, t + k)$  explicitly in terms of the solution at earlier values of time gives

$$\begin{aligned} u(x, t + k) &= 2u(x, t) - u(x, t - k) \\ &+ \left(\frac{k}{h}\right)^2 [u(x + h, t) - 2u(x, t) + u(x - h, t)] \end{aligned} \quad (21.4)$$

- From (21.4) it is clear that we must already know the solution at **two** previous time steps, and, hence, we must use the initial-velocity condition

$$\frac{1}{k} [u(x, k) - \phi(x)] = \psi(x)$$

to get us started. Solving for  $u(x, k)$  gives  $u(x, k) = \phi(x) + k\psi(x)$ , and, thus, we can find the solution for  $t = \Delta t$ .

# An Implicit Finite-Difference Method (Crank-Nicolson Method)

- In implicit method, we again replace the partial derivatives in the problem by their finite-difference approximations, but unlike explicit methods (where we solved for  $u_{i+1,j}$  explicitly in terms of earlier values), in implicit methods, we solve a **system of equations** in order to find the solution at the largest value of time.
- In other words, for each new value of time we solve a system of algebraic equations to find **all** the values.
- It should be mentioned that implicit methods allow us to take larger steps by doing more work per step.

# The Heat-Flow Problem Solved by an Implicit Method

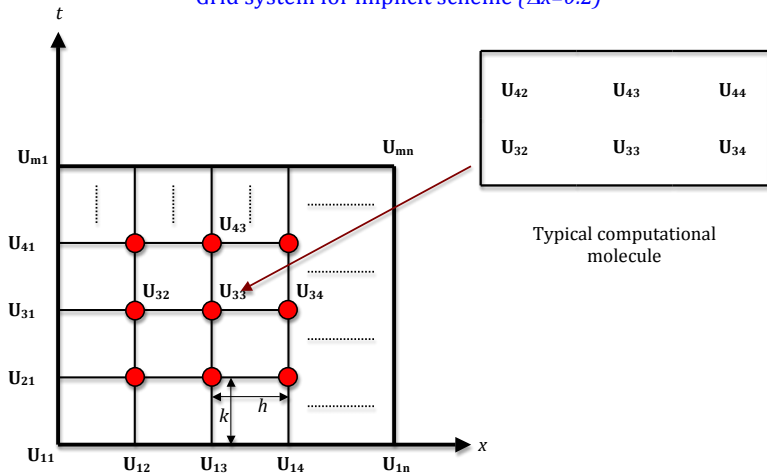
## Problem 21-3

To find a function  $u(x, t)$  that satisfies

$$\text{PDE: } u_t = u_{xx}, \quad 0 < x < 1, \quad 0 < t < \infty$$

$$\text{BCs: } \begin{cases} u(0, t) = 0 \\ u(1, t) = 0 \end{cases} \quad 0 < t < \infty$$

$$\text{IC: } u(x, 0) = 1 \quad 0 \leq x \leq 1$$

Grid system for implicit scheme ( $\Delta x=0.2$ )

- We replace the partial derivatives  $u_t$  and  $u_{xx}$  by the following approximations:

$$u_t(x, t) = \frac{1}{k} [u(x, t + k) - u(x, t)]$$

$$u_{xx}(x, t) = \frac{\lambda}{h^2} [u(x + h, t + k) - 2u(x, t + k) + u(x - h, t + k)] \\ + \frac{(1 - \lambda)}{h^2} [u(x + h, t) - 2u(x, t) + u(x - h, t)],$$

where  $\lambda$  is a chosen number in the interval  $[0, 1]$ .

- Note that our approximation for  $u_{xx}$  is a **weighted average** of the central-difference approximation to the derivative  $u_{xx}$  at time values  $t$  and  $t + k$ .

## Remarks

- In the special case when  $\lambda = 0.5$ , it is just the ordinary average of these two central differences.
- If  $\lambda = 0.75$ , our approximation puts weights of 0.75 and 0.25 on each of the two terms.
- If  $\lambda = 0$ , it is usual **explicit** finite-difference method.

If we now substitute the approximations for  $u_t$  and  $u_{xx}$  into our problem, we get the new **finite-difference problem**

### Problem 21-3a

$$\frac{1}{k} (u_{i+1,j} - u_{i,j}) = \frac{\lambda}{h^2} (u_{i+1,j+1} - 2u_{i+1,j} + u_{i+1,j-1}) + \frac{(1-\lambda)}{h^2} (u_{i,j+1} - 2u_{i,j} + u_{i,j-1})$$

$$\text{BCs: } \begin{cases} u_{i,1} = 0 \\ u_{i,n} = 0 \end{cases}, \quad i = 1, 2, \dots, m$$

$$\text{IC: } u_{1,j} = 1, \quad j = 2, \dots, n-1$$

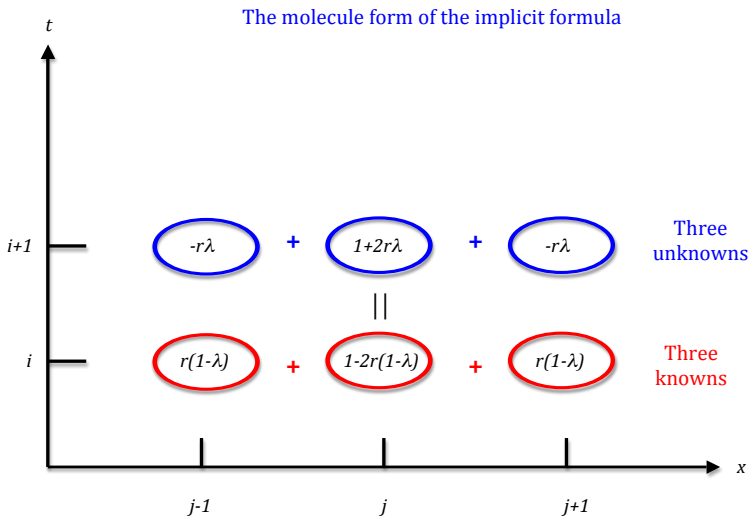


- If we rewrite the difference equation in problem 21-3a, putting the  $u_{i,j}$ 's with the largest time subscript ( $i$ -subscript) on the left-hand side of the equation, we arrive at

$$\begin{aligned}
 -\lambda r u_{i+1,j+1} + (1 + 2r\lambda)u_{i+1,j} - \lambda r u_{i+1,j-1} \\
 = r(1 - \lambda)u_{i,j+1} + [1 - 2r(1 - \lambda)] u_{i,j} \\
 + r(1 - \lambda)u_{i,j-1},
 \end{aligned} \tag{21.5}$$

where we have set  $r = k/h^2$  for convenience.

- Note that for a **fixed subscript  $i$**  and for  $j$  going from 2 to  $n - 1$ , this is a system of  $n - 2$  equations in the  $n - 2$  unknowns  $u_{i+1,2}$ ,  $u_{i+1,3}$ ,  $u_{i+1,4}$ ,  $\dots$ ,  $u_{i+1,n-1}$  [which are the interior grid points at  $t = (i + 1)\Delta t$ ].
- To help show exactly how  $u_{i,j}$ 's are involved into (21.5), we write it in the symbolic or molecular form (see next page)



# Monte Carlo Methods (an Introduction)

- The basic idea here is that **games of chance** can be played (generally on a computer) whose outcomes approximate solutions to real-world problems.
- First of all Monte Carlo methods are procedures for solving **nonprobabilistic-type problems** (problems whose outcome does not depend on chance) by **probabilistic-type methods** (methods whose outcome depends on chance).
- The general philosophy of Monte-Carlo methods is illustrated on the next page.

***Probabilistic game***

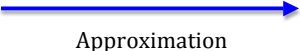
The outcome of the game  $\hat{P}$

(Like the fraction of heads in tossing a coin, throwing darts, and so forth)

***Deterministic problem***

The answer to the problem is  $P$

(Like evaluation an integral, solving a PDE, and so forth)

Outcome =  $\hat{P}$   Answer =  $P$   
Approximation

# Evaluating an Integral

- To illustrate the method, suppose we wanted to evaluate the integral

$$I = \int_a^b f(x) dx$$

(a nonprobabilistic problem).

- To use the Monte Carlo method, we would devise a game of chance whose outcome was the value of the integral (or approximates the integral).
- There are, of course, many games that we could devise; the actual game we used would depend on the accuracy of the approximation, simplicity of the game, and so on.

## Evaluating an Integral (cont.)

- An obvious game to evaluate the integral would be throwing darts at the rectangle

$$R = \{(x, y) : a \leq x \leq b, 0 \leq y \leq \max f(x)\}.$$

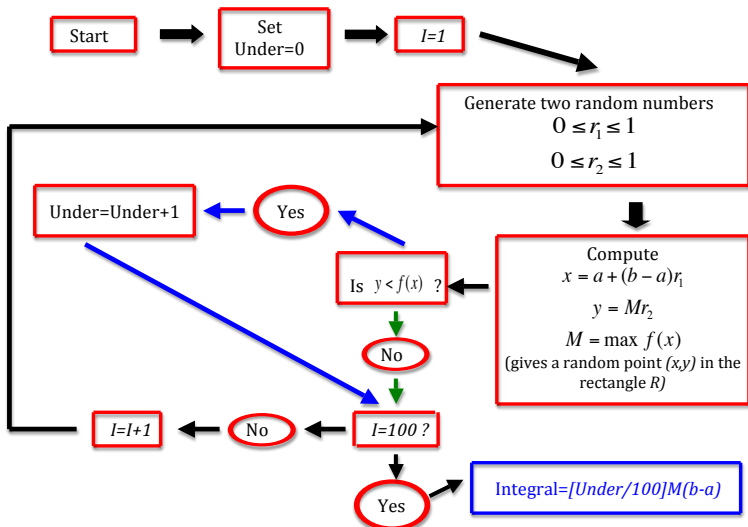
- It's fairly obvious that if we randomly toss 100 or so darts at the rectangle  $R$  enclosing the graph, then the fraction of darts hitting below the curve times the area of  $R$  will estimate the value of the integral.
- Hence, our outcome of the game

$$\hat{I} = [\text{fraction of tosses under } f(x)] \times (\text{area of } R)$$

is used to estimate the true value of the integral  $I$ .

## Evaluating an Integral (cont.)

- To carry out the actual computation on a computer, we would have to generate the sequence of random points in some way (we'll discuss this shortly) and have the computer play the dart tossing game.
- Let us assume for the time being that we have a sequence of random points. The flow diagram on the next page illustrates how the computer would attack this problem. (See flow diagram to evaluate  $\int_a^b f(x)dx$  by the Monte Carlo method (100 tosses)).





# Random Numbers

- Before going on to apply this technique to the solution of PDEs, we discuss the important topic of random numbers.
- In the integral just considered, it was necessary to generate a sequence of random points  $P_i = (x_i, y_i)$  that fell inside rectangle  $R$ . In other words, the  $x$ -coordinate would have to be a random number in the interval  $[a, b]$ , while  $y_i$  must be in  $[0, M]$ .

## Random Numbers (cont.)

- To find random numbers inside specific intervals, we start with a basic sequence of random numbers  $r_i$  (uniformly distributed) inside  $[0, 1]$ .
- It's obvious then that if we want a random number  $x_i$  inside  $[a, b]$ , we just compute

$$x_i = a + (b - a)r_i$$

- So everything comes down to the question, how do we generate a sequence of random numbers  $\{r_i, i = 1, 2, \dots\}$  uniformly distributed in  $[0, 1]$ .

# Residue Algorithm for Generating Random Numbers

To generate a sequence of **random integers** (between 0 and  $P$ ), we use the **residue algorithm**.

- 1 Pick the first random integer any way you like between 0 and  $P$  ( $P$  was picked in advance).
- 2 Multiply this random integer by some fixed integer  $M$  (picked in advance).
- 3 Add to that product another fixed integer  $K$  (picked in advance).
- 4 Divide the resulting sum by  $P$  and pick the **remainder** as the new random integer. Now go back to step 2 and repeat steps 2-4 until you have enough random integers.

- This residue algorithm can be written as

$$r_{i+1} \equiv (Mr_i + K) \bmod P \quad i = 0, 1, 2, \dots$$

which says, if we are given a random integer  $r_i$ , then to compute a new one  $r_{i+1}$ , we multiply by  $M$ , add  $K$ , divide by  $P$ , and pick the remainder.

## Remarks

- If we choose, for example,  $P = 100$  in our random-number generator, the remainders will be one of the integers  $0, 1, 2, \dots, 99$ , and, hence, our entire process will start repeating before long.
- In fact, our random numbers might be

15, 71, 43, 7, 43, 7, 43, 7,      (Cycle of two numbers)

and, hence, our method is no good.

- The ideal situation is to generate the entire residue class  $\{0, 1, 2, \dots, 99\}$  in a **random fashion** before starting to repeat.

## Remarks (cont.)

- It can be proven mathematically that if the numbers  $M$ ,  $K$ , and  $P$  are chosen according to certain rules, then no matter how we pick the first random number  $r_0$ , the algorithm will generate the entire residue class.
- So, if we pick  $P$  very large (like  $2^{40}$ ), we are assured that (for practical purposes) the process will never repeat.
- It is possible to generate random samples from various statistical distributions other than the uniform distribution  $f(x) = 1$ ,  $0 < x < 1$  (the usual random-generator).
- Computer programs are available to generate random samples from the binomial, gamma, normal, and many other distributions.

# Monte Carlo Solution of PDEs

We show how we can design a game to approximate solution of the Dirichlet problem:

## Problem 21-4

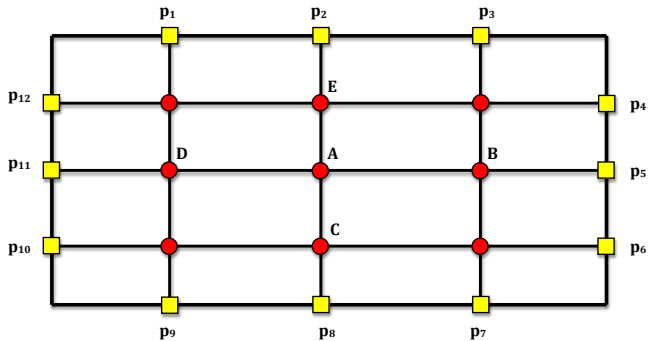
To find a function  $u(x, y)$  that satisfies

$$\text{PDE: } u_{xx} + u_{yy} = 0, \quad 0 < x < 1, \quad 0 < y < 1$$

$$\text{BC: } u(x, y) = g(x, y) = \begin{cases} 1, & \text{On the top of the square} \\ 0, & \text{On the sides and} \\ & \text{bottom of the square} \end{cases}$$

To illustrate the Monte Carlo method in this problem, we introduce a game called **tour du wino**. To play it, we need a board on which grid lines are drawn (see next page).

## Board for tour du wino



A = starting points for game

■ = end points  $p_i$

● = interior grid points

$g_i$  = reward for ending at  $p_i$



# How Tour du Wino is Played

1. The wino starts from an arbitrary point (point  $A$  in our case).
2. At each stage of the game, the wino staggers off randomly to one of the four neighboring points. (In our case, the neighbors of  $A$  are  $B$ ,  $C$ ,  $D$  and  $E$ , and the probability of going to each of these neighbors is  $1/4$ ).
3. After arriving at a neighboring point, the wino continues this process wandering from point to point until eventually hitting a **boundary point**  $p_j$ . He then stops, and we record that point  $p_j$ . This completes one **random walk**.

## How Tour du Wino is Played (cont.)

4. We repeat steps 1-3 until many random walks are completed. We now compute the fraction of times the wino had ended up at each of the boundary points  $p_i$ .
5. Suppose the wino receives a reward  $g_i$  ( $g_i$  is the value of the BC at  $p_i$ ) if he ends his walk at the boundary point  $p_i$ , and suppose that the goal of the game is to compute his average reward  $R(A)$  for all this walks. The average reward is

$$R(A) = g_1 P_A(p_1) + g_2 P_A(p_2) + \cdots + g_{12} P_A(p_{12})$$

The game is completed with the determination of  $R(A)$ .

# Probability of Random Walk Ending at $p_i$

Boundary point $p_i$	$P_A(p_i)$ = fraction of times the wino ends at $p_i$	$g_i$ = reward for ending at $p_i$
1	0.04	1
2	0.15	1
3	0.03	1
4	0.06	0
5	0.17	0
6	0.05	0
7	0.06	0
8	0.15	0
9	0.03	0
10	0.06	0
11	0.16	0
12	0.04	0

# Reason for Playing Tour du Wino

It turns out that the average reward is the approximate solution to our Dirichlet problem at Point  $A$ . This interesting observation is based on two facts.

- 1 Suppose the wino started at a point  $A$  that was on the **boundary** of the square. Each resulting random walk ends immediately at that point, and the wino collects the amount  $g_j$ . Thus, his average reward for starting from a boundary point is also  $g_j$ .
- 2 Now suppose the wino starts from an interior point. Then, the average reward  $R(A)$  is clearly the average of the four average rewards of the four neighbors

$$R(A) = \frac{1}{4} [R(B) + R(C) + R(D) + R(E)]$$

- We ask why the wino's average reward  $R(A)$  approximates the solution of the Dirichlet problem at  $A$ . We have seen that  $R(A)$  satisfies two equations

$$R(A) = \frac{1}{4} [R(B) + R(C) + R(D) + R(E)] \quad (A \text{ an interior point})$$

$$R(A) = g_i \quad (A \text{ a boundary point})$$

- If we let  $g_i$  be the value of the boundary function  $g(x, y)$  at the boundary point  $p_i$ , then our two equations are exactly the two equations we arrived at when we solved the Dirichlet problem by the finite-difference method.

- That is,  $R(A)$  corresponds to  $u_{i,j}$  in the finite-difference equations

$$u_{i,j} = \frac{1}{4} (u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}) \quad (i,j) \text{ an interior point}$$

$$u_{i,j} = g_{i,j} \quad g_{i,j} \text{ the solution at a boundary point } (i,j)$$

- Hence,  $R(A)$  will approximate the true solution of the PDE at  $A$ .

# Solution of Laplace's Equation by the Monte Carlo Method

These rules give the solution at one point inside the square.

1. Generate several random walks starting at some specific point  $A$  and ending once you hit a boundary point. Keep track of how many times you hit each boundary point.
2. After completing the walks, compute the fraction of times you have ended at each point  $p_i$ . Call these fractions  $P_A(p_i)$ .
3. Compute the **approximate solution**  $u(A)$  from the formula

$$u(A) = g_1 P_A(p_1) + g_2 P_A(p_2) + \cdots + g_N P_A(p_N)$$

where  $g_i$  is the value of the function at  $p_i$  and  $N$  is the number of boundary points.

# Solution to a Dirichlet Problem with Variable Coefficients

The game tour du wino can be modified to solve more complicated problems, as in the following example.

## Problem 21-5

To find a function  $u(x, y)$  that satisfies

$$\text{PDE: } u_{xx} + (\sin x) u_{yy} = 0, \quad 0 < x < \pi, \quad 0 < y < \pi$$

$$\text{BC: } u(x, y) = g(x, y) \quad \text{on the boundary of the square}$$



- To solve Problem 21-5, we replace  $u_{xx}$ ,  $u_{yy}$  and  $\sin x$  by

$$u_{xx} = [u_{i,j+1} - 2u_{i,j} + u_{i,j-1}] / h^2$$

$$u_{yy} = [u_{i+1,j} - 2u_{i,j} + u_{i-1,j}] / k^2$$

$$\sin x = \sin x_j$$

and plug them into the PDE.

- Making these substitutions and solving for  $u_{i,j}$  gives

$$u_{i,j} = \frac{u_{i,j+1} + u_{i,j-1} + \sin x_j (u_{i+1,j} + u_{i-1,j})}{2(1 + \sin x_j)} \quad (21.6)$$

- Look carefully at (21.6). The coefficients of  $u_{i+1,j}$ ,  $u_{i-1,j}$ ,  $u_{i,j+1}$ , and  $u_{i,j-1}$  are positive and sum to one. In other words,  $u_{i,j}$  is a **weighted average** of the solutions at the four neighboring points.
- Hence, we modify our game so that the wino doesn't stagger off to each neighbor with probability  $1/4$ , but, rather, with a probability equal to the coefficients of the respective term.

- In other words, if the wino is at the point  $(i, j)$ , he then goes to the point:

$$(i, j + 1) \text{ with probability } \frac{1}{2(1 + \sin x_j)}$$

$$(i, j - 1) \text{ with probability } \frac{1}{2(1 + \sin x_j)}$$

$$(i + 1, j) \text{ with probability } \frac{\sin x_j}{2(1 + \sin x_j)}$$

$$(i - 1, j) \text{ with probability } \frac{\sin x_j}{2(1 + \sin x_j)}$$

- Other than this slight modification, the game is exactly the same as before.

## Remarks

- Observe that once the fractions  $P_A(p_i)$  (the fraction of times the wino ends at  $p_i$ ) are computed, we can then find the solution  $u(A)$  for any other boundary conditions  $g_i$  just by plugging the  $P_A(p_i)$  into the formula

$$u(A) = g_1 P_A(p_1) + g_2 P_A(p_2) + \cdots + g_N P_A(p_N).$$

That is, we don't have to recompute new random walks.

- In many cases, a researcher wants to find the solution of a PDE at only one point. If the boundary is fairly complicated and if the PDE involves 3 or 4 dimensions, then Monte Carlo methods may come to rescue.

## Remarks (cont.)

- In fact, Monte Carlo methods were originally developed to study difficult neutron-diffusion problems that were impossible to solve analytically.