MIXED BOUNDARY VALUE PROBLEMS

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INTRODUCTION

Mixed boundary value problems are practical situations that are met in most potential and other mathematical physics problems. In this case the boundaries can have values of the functions specified on them as a Dirichlet boundary condition, and derivatives as Neumann boundary conditions. The Neumann problem is to find a function u that is defined, continuous, and differentiable over a closed domain D with boundary C with reflective boundary conditions that could represent insulated adiabatic boundaries, unit cell boundaries, partially reflective or actual normal, specular reflection, or diffusive boundary conditions. For Laplace's equation, a mixed boundary value problem, could also have a combination of the function and its derivative defined at the boundary C:

$$\begin{aligned} &\nabla^2 u = 0 \ on \ D, \\ &u = (af + b\frac{df}{dr}) \ on \ C, \end{aligned} \tag{1}$$

where: f is some prescribed function, $\frac{df}{dr}$ is its derivative, a and b are constants, and ∇^2 is the Laplacian operator.

A random walk that is generated starting from an inner point and moving to the boundary, determines the solution at the starting point. One can visualize the random walk as a stepwise trip undertaken by a drunken person walking in a city, heading at intersection north, south, east or west randomly with equal probability, his walk stopping when he reaches the city wall or boundary, or continuing his walk by being reflected back into the city, depending on whether the walls are absorbing or reflecting..

ANALYTICAL SOLUTION BENCHMARK

When Monte Carlo simulations are first undertaken, it is always useful to check the results of the algorithm against some benchmark. The benchmark would normally solve a simpler problem for which an analytical solution can be derived. One could also use the solution generated by another numerical method. Best, the Monte Carlo simulation should be compared to the experimental results of a simple problem before applying the Monte Carlo model to more complex problems that may not lend themselves to an analytical solution, a numerical solution by other methods, or experimental verification. Faced by a Monte Carlo simulation that does not adequately predict the results of a complex experiment, a Monte Carlo practitioner cannot blame the experiment or the real world for not matching the predictions of his procedure. He has only himself to blame for not thoroughly testing his model before applying it in the real world.

To illuminate the way towards avoiding such pitfalls, we suggest a simple benchmark for which an exact analytical solution can be easily derived. We build the Monte Carlo model that can solve this analytical solution. With our acquired confidence, we can then apply our procedure to problems of mixed boundary conditions that neither possess analytical or numerical solutions nor experimental results.

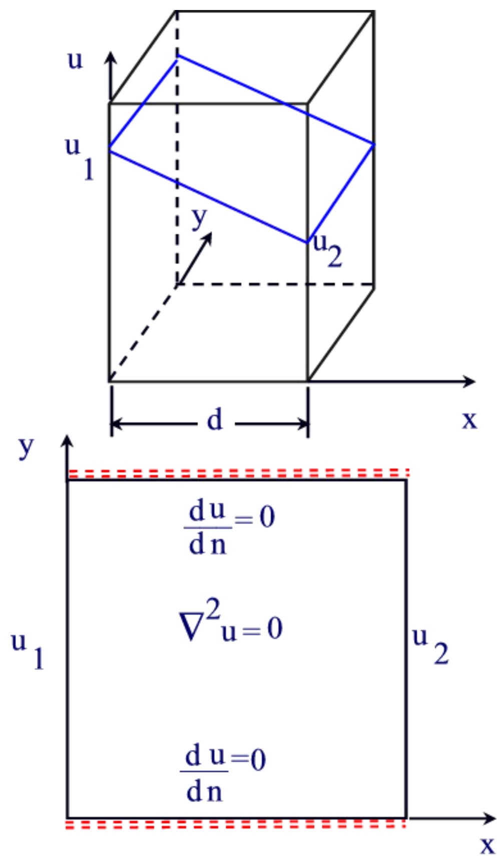

Figure 1. Two-dimensional potential problem with mixed Dirichlet and Neumann boundary conditions.

We consider the two-dimensional square plate of side length d shown in Fig. 1. We consider a set of boundary conditions of the mixed type in the sense that some boundaries have Dirichlet type conditions, whilst other boundaries have Neumann boundary conditions specified on them. In particular, let the left and right boundaries have Dirichlet boundary conditions, while the top and bottom boundaries have Neumann boundary conditions.

Practically, this problem could represent a plate heated at the left hand side to a temperature u_1, while the right hand side boundary is cooled and maintained at a temperature u_2. The top and bottom sides are insulated and constitute adiabatic insulated boundaries with no heat flux flowing through them.

Alternatively, the square plate could represent an electrical conductor maintained at a voltage u_1 on the left side and grounded on the right hand side to a voltage u_2, with no current flow across the top and bottom boundaries, which are insulated.

Another possibility is the representation of liquid flow through a homogeneous porous medium, from the left hand side that is maintained at a hydrostatic head u_1 to a sink on the right hand side maintained at a hydrostatic head u_2 with the top and lower boundaries composed of impervious soil profile that do not allow liquid flow through the top or bottom boundaries.

For a homogeneous medium with uniform properties, the underlying governing equation is the Laplace Equation. Because of the problem's symmetry along the y axis, with the derivative to the solution zero everywhere, the solution along the y axis is a constant everywhere and the equation needs only to be solved along the x axis. Consequently we can write:

$$\nabla^2 u = \frac{d^2u}{dx^2} = \frac{d}{dx}\left(\frac{du}{dx}\right) = 0 \tag{2}$$

Integrating once:

$$\int d\left(\frac{du}{dx}\right) = 0 \ , \Rightarrow \frac{du}{dx} = a \tag{3}$$

where a is an integration constant.

Integrating a second time, we get:

$$\int du = \int a \ dx \ , \Rightarrow u = ax + b \tag{4}$$

Applying the two boundary conditions:

$$\begin{aligned} u &= u_1 \ \ for \ x = 0 \ , \\ u &= u_2 \ \ for \ x = d \ . \end{aligned} \tag{5}$$

yields:

$$\begin{aligned} b &= u_1 \ , \\ a &= \frac{(u_2 - u_1)}{d} \end{aligned} \tag{6}$$

Substituting from Eqn. 6 into Eqn. 4 we get:

$$u(x) = u_1 - \frac{(u_1 - u_{2)}}{d} \ x \tag{7}$$

which is the equation of a straight line of negative slope $\frac{(u_1 - u_2)}{d}$, intersecting the y axis at u_1.

MONTE CARLO PROCEDURE

The previous procedure developed for Dirichlet boundary conditions, is here developed for mixed type of Dirichlet and Neumann boundary conditions as shown in Fig. 2. Scoring the boundary value whenever the random walk reaches the boundary is commented out and replaced by a reflection of the particle back to its original position whenever it reaches a reflecting boundary.

The solution is stored either as an Excel file or an Array Visualizer file, depending on which visualization option will be used. The rest of the features remain the same as in the original Dirichlet implementation. Depending on the problem at hand, the boundary conditions can be modified accordingly. If the medium is not homogeneous, the transition probabilities can be easily modified.

First, the procedure adequacy will be tested against the derived benchmark, for which we know the exact analytical solution. Only then can we proceed to apply the procedure to a problem whose analytical, or even numerical solution would be hard to obtain otherwise.

```
!       Laplace_solver_profile_mixed for
        program Laplace_solver_profile_mixed
!       Two-dimensional Laplace's Equation Solver, with profile generation
!       Laplace's Equation in two Dimensions, Cartesian Coordinates.
!       Solution by Monte Carlo random walk on a rectangular surface
!       with mixed Dirichlet and Neumann boundary conditions
!       M. Ragheb
!       Random walk with equal step sizes
        dimension score(31,31), temp(31,31)
        real(8) elapsed_time
        character*1 tab
        elapsed_time=timef()
        tab=char(9)
!       Store output matrix for visualization using Excel
!       open (unit=10, file='temp_profile.xls', status='unknown')
!       Store output matrix for visualization using the Array visualizer
        open (unit=10, file='temp_profile.agl', status='unknown')
!       m1 = number of mesh points in x-direction
        m1=31
!       n1 = number of mesh points in y-direction
        n1=31
!       step probabilities in x+:p1, y+:p2, x-:p3 and y-:p4 directions
        p1=0.25
        p2=0.25
        p3=0.25
        p4=0.25
!       Construct cumulative distribution function for random walk
        p12=p1+p2
        p123=p1+p2+p3
!       number of random walks: nsamp
        nsamp=100
!       Boundary conditions on the rectangle
!       left t1=t(0,y), bottom t2=t(x,0), right t3=t(m1,y), upper t4=t(x,n1)
        t1=100.
        t2=0.
        t3=0.
        t4=0.
!       Coordinates indices of point at which solution is estimated
```

```
!       m: i0=x/dx, n: j0=y/dy
        do 30 m=2,30,1
        do 30 n=2,30,1
!       m=11
!       n=11
!       Start random walk here
!       Initialize counters
!       History counter
        ncount=0
!       Score counter
        score(m,n)=0.0
!       Initiate random walk
99      i=m
        j=n
999     call random(r)
!       Sample cumulative distribution function for random walk
!       Move one step to the right
        if (r le.p1) then
        i=i+1
        goto 11
!       Move one step up
        else if (r le.p12) then
        j=j+1
        goto 11
!       Move one step left
        else if (r le.p123) then
        i=i-1
        goto 11
        else
!       Move one step down
        j=j-1
        goto 11
        end if
!       Check for random walk reaching boundary
!       Check whether lower boundary is reached
11      if (j.eq.1) then
!       score(m,n) = score(m,n) + t2
!               Reflective boundary condition
        j=j+1
!       goto 88
!               Continue random walk, do not terminate history
        goto 999
!       Check whether right boundary is reached
        else if (i.eq m1) then
        score(m,n) = score(m,n) + t3
        goto 88
!       Check whether upper boundary is reached
        else if (j.eq n1) then
!       score(m,n) = score(m,n) + t4
!               Reflective boundary condition
        j=j-1
!       goto 88
!               Continue random walk, do not terminate history
        goto 999
!       Check whether left boundary is reached
        else if (i.eq.1)  then
        score(m,n) = score(m,n) + t1
!       write(*,*) score
        goto 88
        else
        goto 999
        end if
```

```
!       Increment history counter
88      ncount=ncount+1
!       Check for total number of histories
        if (ncount lt nsamp) then
        goto 99
        else
        goto 77
        end if
!       Calculate solution at points of interest
77      xcount=ncount
        temp(m,n)=score(m,n)/xcount
!       write(10,*) temp(m,n)
!       write(*,*) score
!       write(*,*) xcount
!       Print results
30      continue
        write(*,*)'number of random walks=',nsamp
!       write(*,*)'coordinate of point at which temperature is calculated',m,n
!       write(*,*)'calculated temperature=',temp
        write(*,300) temp
!       Boundary values
        do 40 i=1,31
                do 40 j=1,31
!               bottom boundary
!               temp(i,1)=0.0
!               top boundary
!               temp(i,31)=0.0
!               left boundary
                temp(1,j)=100.0
!               right boundary
                temp(31,j)=0.0
40      continue
        do 20 n=1,31
        write(10,300) (temp(m,n),tab, m=1,31)
20      continue
300     format(31(e14.8,a1))
!       elapsed_time=timef()
        write(*,*) elapsed_time
!       stop
        end
```

Figure 2. Random walk Monte Carlo procedure showing modification for the treatment of mixed Dirichlet and Neumann boundary conditions.

BENCHMARK MONTE CARLO RESULTS

To test the Monte results against the analytical benchmark, we use the following boundary conditions:

$$u_1 = 100 \text{ , } at \;\; x = 0,$$

$$u_2 = 0 \quad \text{ , } at \;\; x = d,$$

$$\frac{du}{dy} = 0 \quad \text{ , } at \;\; y = 0 \text{ , } y = d.$$

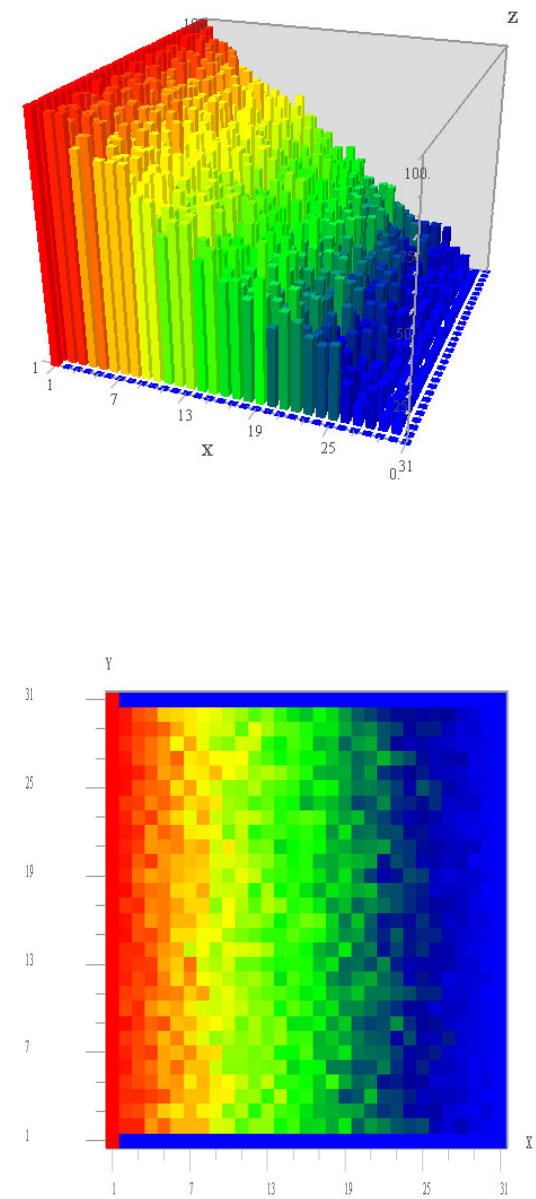

Figure 3. Temperature profile, N=100 random walks per node.

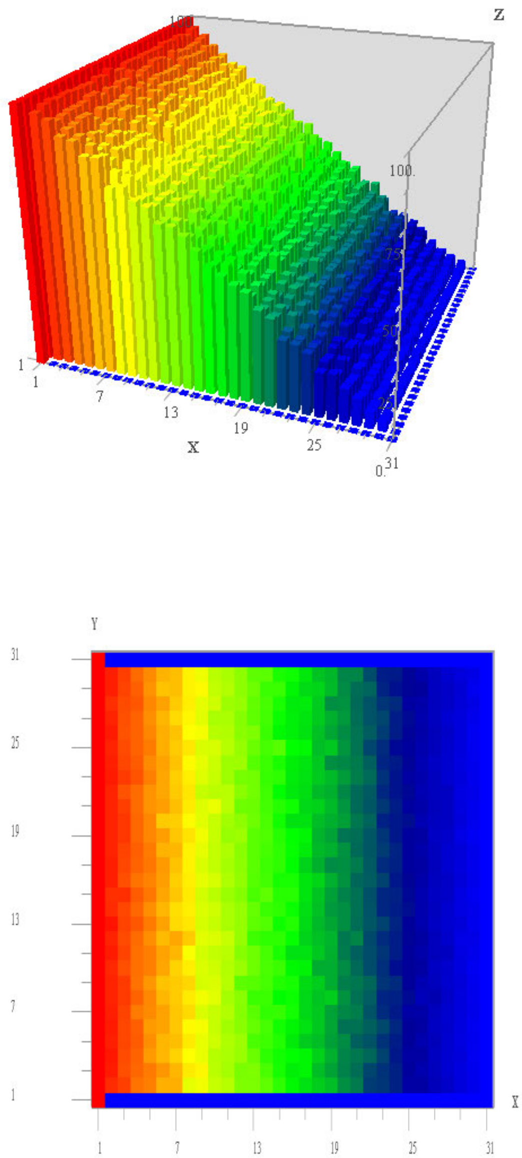

Figure 4. Temperature profile, N=1,000 random walks per node.

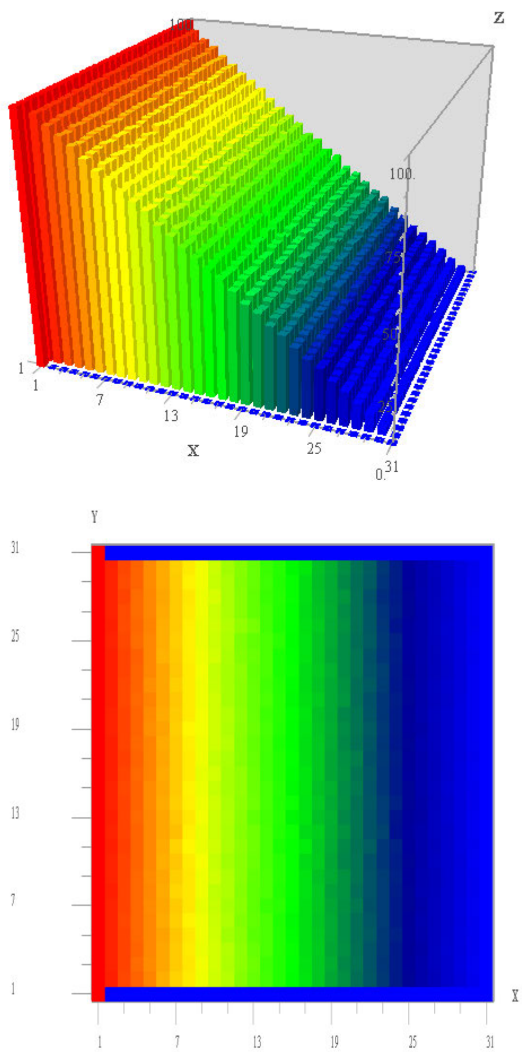

Figure 5. Temperature profile, N=10,000 random walks per node.

The simulation results are displayed in Figs. 3, 4 and 5 in histogram form at each random walk node point. The agreement with the straight-line exact analytical solution is remarkable even at a small number of random walks per node. Figure 3 shows the simulation results for N=100 generated random walks per node. Both a height and a planar result are displayed using the Array Visualizer. Plotting of the results is in terms of the rainbow colors where red implies a higher value or hot value of the parameters, and blue a lower or cooler magnitude.

To study the effect of the number of histories, we increased the value of N to 1,000, and then to 10,000 with the results shown in Figs. 4 and 5. One notices a dramatic improvement in the estimates of the simulation when moving to a higher number of histories. The execution times are relatively modest and were carried out on a laptop platform with a Pentium III processor. One notices a linear increase in the execution time as the number of random walks per node is increased as shown in Table 1.

Table 1. Execution times for benchmark for different random walks generated per node.

Random walks per node N	Execution time [seconds]
10^2	3.5
10^3	33.8
10^4	339.5

A MIXED DIRICHLET AND NEUMANN BOUNDARY VALUE PROBLEM

Having acquired confidence in the efficacy of the Monte Carlo procedure for solving such a class of problems, we are now able to apply it to a problem for which deriving an analytical solution would not be an easy task.

The geometry of the problem is shown in Fig. 6, and the Monte Carlo simulation result for N=10,000 are shown in Fig.7.

The problem represents a square domain with a potential, temperature, or hydrostatic head applied to the left boundary, with a heat sink, electrical ground or fluid sink at the right and bottom boundaries. The top boundary represents a heat or electrically insulated or an impervious medium boundary medium. This otherwise heat transport, electrical potential or hydrostatic problem is mathematically speaking a mixed Dirichlet and Neumann boundary condition problem.

The result from the Monte Carlo random walk procedure in Fig. 7 shows that the boundary conditions are well satisfied close to the boundary. It is also remarkable to notice the local influence of the boundary conditions on the result. Close to the insulated top boundary, the result appears as a straight line, which smoothly turned into a curved solution that decreases from the left boundary representing the source to the right and bottom boundaries representing the sink.

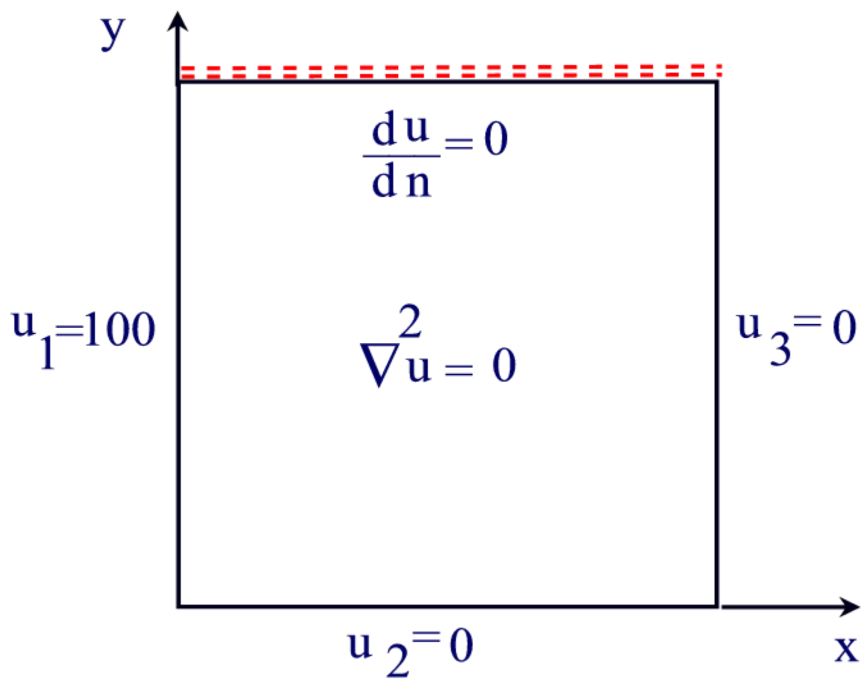

Figure 6. Geometry and boundary conditions for mixed type Dirichlet and Neumann boundary conditions.

DISCUSSION

The Monte Carlo method offers a valuable tool for the treatment of the class of problems encountered in science and engineering where the boundary conditions are of the mixed Dirichlet and Neumann types. Analytical solutions could be hard to derive, and other numerical solutions may not be able to deal with non-linearity and higher dimensions. When Monte Carlo simulations are first undertaken, it is recommended to check the results of the generated algorithm against a benchmark of choice. The benchmark would normally solve a simpler problem for which an analytical solution can be derived. One could also use the solution generated by another numerical method. Best, the Monte Carlo simulation should be compared to any available experimental results.

It is facetious to suggest, when a Monte Carlo code does not match the results of a physical experiment, that the experiment or its measurements are to blame. How could the humble experiment not match the elegant and dazzling Monte Carlo code that took so much effort to write, but not to test, and that was also run on the latest, most expensive and most powerful supercomputer?

The real world cannot be blamed for the deficiency and the lack of checking of a Monte Carlo procedure against some simple benchmarks before applying it to real world problems.

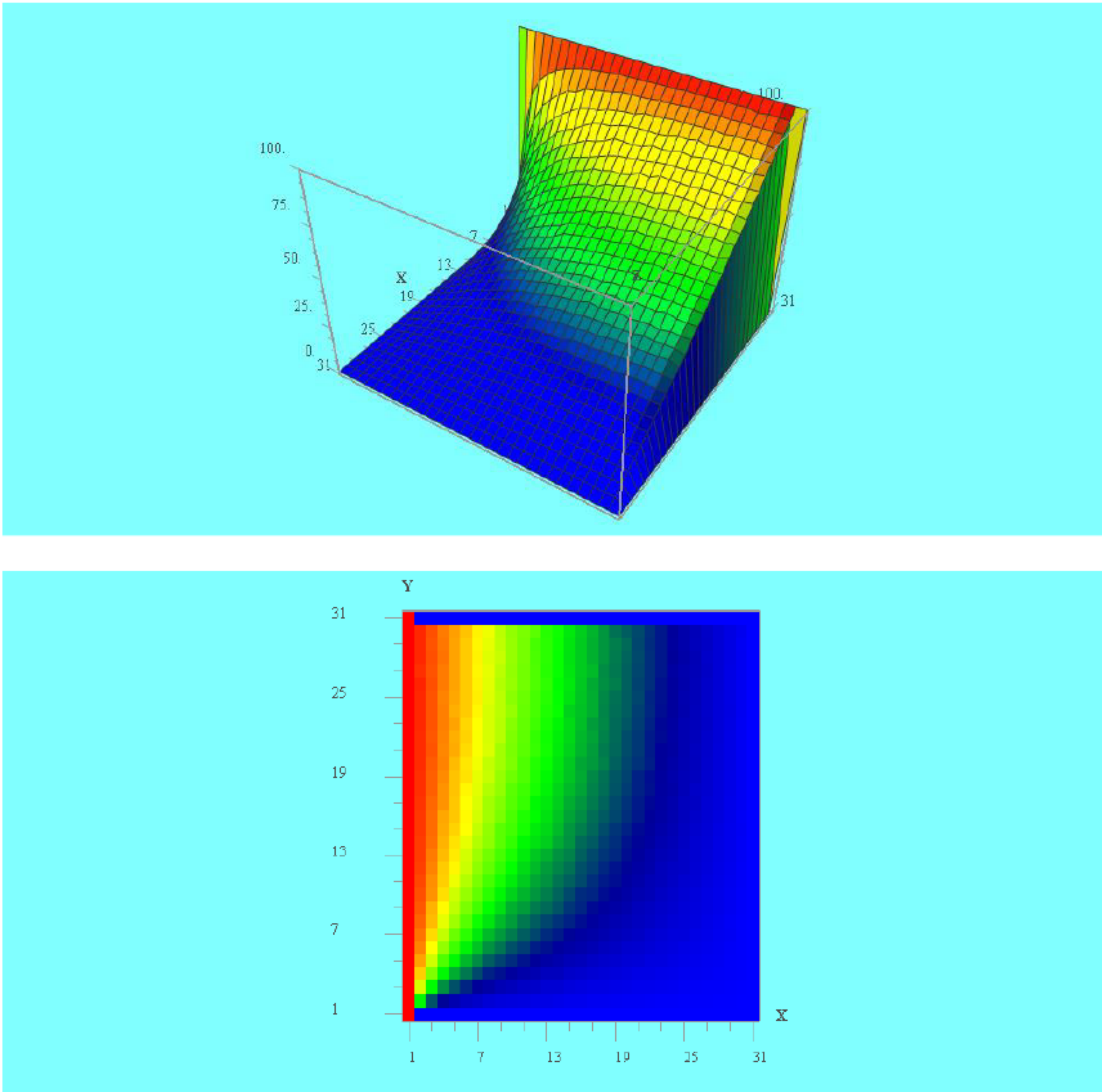

Figure 7. Temperature profile for mixed type Dirichlet and Neumann boundary conditions, N=10,000 random walks.

PROBLEMS

1. In mixed Dirichlet-Neumann boundary value problems, a single boundary can have both types of boundary conditions imposed on it. Modify the procedure to seek solutions where part of a boundary has the value of the function specified, and another part of the boundary has a reflective boundary condition or the derivative specified on it.
2. Modify the procedure to allow for a triangular mesh. In this case the particle can move in six different directions instead of four in the plane, allowing for better representation of reflection at reflective boundaries.
3. Write a procedure to solve the benchmark problem with the exact analytical solution using a floating random walk in the plane. Whence the algorithm is tested against the benchmark, try extending to a three dimensional system.
4. Other types of reflective boundary conditions can be specified other than the normal reflection. Modify the procedure to allow for a diffusive type of reflection. If you could use a floating walk, you could also implement a specular reflection condition.
5. Simulate the flow of oil or natural gas from an oil reservoir into an oil well that extends only half the way through the reservoir. Consider the top and bottom of the reservoir as reflecting boundaries. Take the right boundary of a rectangular surface to be at a reference hydrostatic potential, with the well approximated as a line sink covering half the top of the left boundary, with the rest of it as a reflecting boundary.