Methods of Computational Physics - I (PHY637MJ)

Internal Examination

Ayush Shenoy (24021014)

December 2025

Question 2

Code:

```
! AYUSH SHENOY
! 24021014
! INTERNAL EXAM (QUESTION 2)

program DICE

    implicit none

    real::ROLL(4)
    integer::I,J,N
    real::M,SQM
    read(*,*) N

    M = 0
    SQM = 0

    do I=1,N
        call RANDOM_NUMBER(ROLL)
        ROLL = ceiling(ROLL*6)
        write(*,*) (ROLL(J), J=1,4)
        M = M + ROLL(1)
        SQM = SQM + ROLL(1)**2
    end do

    M = M/N
    SQM = SQM/N

    write(*,*) "Mean: ", M
    write(*,*) "Uniform mean: ", 3.5
    write(*,*) "Var :" , SQM - M**2
    write(*,*) "Uniform Var", 2.917

end program DICE
```

Output:

Sample output for $n = 10$

```
2       1       1       5
1       6       6       4
5       6       3       3
4       6       1       5
4       1       1       1
1       4       5       2
6       3       1       1
6       3       3       1
5       6       4       2
3       3       1       6
```

```
 Mean:    3.70000005
 Uniform mean:    3.50000000
 Var :   3.20999908
 Uniform Var   2.91700006
```

For $n = 100000$:

```
Mean:    3.50481009
Uniform mean:    3.50000000
Var :   2.92839527
Uniform Var   2.91700006
```

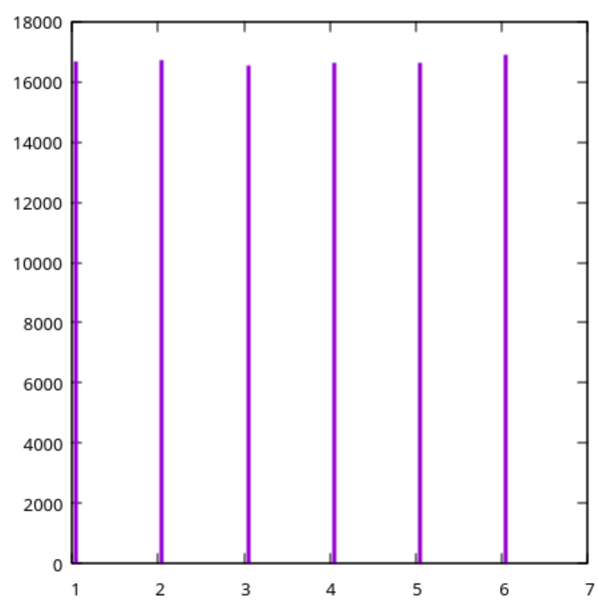

Figure 1: Histogram plotted for $n = 100000$

Question 3

We are tasked with evaluating the expectation value of the Coulomb interaction in the ground state of the Helium atom, expressed in spherical polar coordinates:

$$I = \int_{r_1=0}^{\infty} \int_{r_2=0}^{\infty} \int_{\theta_1=0}^{\pi} \int_{\theta_2=0}^{\pi} \int_{\phi_1=0}^{2\pi} \int_{\phi_2=0}^{2\pi} r_1^2 e^{-4r_1} r_2^2 e^{-4r_2} \sin\theta_1 \sin\theta_2 \frac{1}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\beta}} dr_1 dr_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2$$

where

$$\cos\beta = \cos\theta_1 + \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\phi_1 - \phi_2)$$

We note that the integral has a sharp inverse exponential dependence on r_1 and r_2, making exponential sampling desirable for the radial co-ordinates. For the angular co-ordinates, we use uniform sampling over their domain.

To sample from the exponential distribution, we use the Inverse-CDF method. Consider the PDF

$$f_X(x) = \begin{cases} 4e^{-4x} & x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

The corresponding CDF is

$$F_X(x) = \begin{cases} 1 - e^{-4x} & x \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

The inverse CDF in terms of a uniformly distributed random variable Y is then

$$F_Y^{-1}(y) = \begin{cases} -\frac{1}{4} \ln(1-y) & 0 \leq y \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

Since all the random variables are independent of each other, the joint PDF is simply the product of the individual PDFs:

$$f(r_1, r_2, \theta_1, \theta_2, \phi_1, \phi_2) = \frac{4}{\pi^4} e^{-4(r_1 + r_2)}$$

Define

$$g(r_1, r_2, \theta_1, \theta_2, \phi_1, \phi_2) = \frac{r_1^2 r_2^2 \sin\theta_1 \sin\theta_2}{\sqrt{r_1^2 + r_2^2 - 2r_1 r_2 \cos\beta}}$$

The integral is then (with aforementioned limits implied)

$$\begin{aligned} I &= \frac{\pi^4}{4} \int f(r_1, r_2, \theta_1, \theta_2, \phi_1, \phi_2) g(r_1, r_2, \theta_1, \theta_2, \phi_1, \phi_2) dr_1 dr_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2 \\ &= \frac{\pi^4}{4} \langle g \rangle \end{aligned}$$

Code:

```
! AYUSH SHENOY
! 24021014
! INTERNAL EXAM (QUESTION 3)

subroutine RAND_EXP(X,LAMBDA)
    ! Sample exponential distribution with mean LAMBDA

    real, intent(inout) :: X
    real, intent(in)    :: LAMBDA

    call RANDOM_NUMBER(X)
    X = 1.0 - X
    X = - log(X)/LAMBDA

end subroutine

subroutine MC_TRIAL(N,M,ENSAV,ENSERR)

    ! Conduct MC trial of M experiments, each with N throws

    integer, intent(in) :: N
    integer, intent(in) :: M
    real, intent(out)   :: ENSAV
    real, intent(out)   :: ENSERR

    integer         :: I,J
    real            ::  R1,R2,T1,T2,P1,P2,CBETA,DENOM
    real,parameter  :: PI = acos(-1.0)
    real            :: ENS(M)

    ENSAV = 0
    ERR = 0

    do J = 1,M

        ESTIMATE = 0
        I = 1

        do while (I<N)
            ! Sample random variables
            call RAND_EXP(R1,4.0)
            call RAND_EXP(R2,4.0)
            call RANDOM_NUMBER(T1)
            call RANDOM_NUMBER(T2)
            call RANDOM_NUMBER(P1)
            call RANDOM_NUMBER(P2)
            T1 = PI*T1
            T2 = PI*T2
            P1 = 2*PI*P1
            P2 = 2*PI*P2
```

```
            ! Calculate integrand
            CBETA = cos(T1) + cos(T2) + sin(T1)*sin(T2)*cos(P1-P2)
            DENOM = R1**2 + R2**2 - 2*R1*R2*CBETA
            DENOM = sqrt(DENOM)

            ! If not divergent, compute expectation value
            if (DENOM > 1E-2) then
                ESTIMATE = ESTIMATE + (R1**2)*(R2**2)*sin(T1)*sin(T2)/DENOM
                I = I + 1
            end if
            end do
            ENS(J) = (0.25*PI**4)*ESTIMATE/N
    end do
    ENSAV = sum(ENS)/M

    ENS = ENS - ENSAV
    ENSERR = sqrt(sum(ENS**2)/(real(M)*(real(M)-1)))

end subroutine MC_TRIAL

program CORREL

    implicit none

    integer :: N ! Number of throws in a experiment
    integer :: M ! Number of experiments in an ensemble
    real    :: INTEG
    real    :: ERR

    N = 100000    ! Reasonably large

    call MC_TRIAL(N,1,INTEG,ERR)
    write(*,*) "Result for 1 trial : ", INTEG
    write(*,*)

    ! Run MC simulation
    write(*,"(A4,4X,3(A15,4X))") "M", "1/SQRT(M)", "INTEGRAL", "ERROR"
    write(*,"(A4,4X,3(A15,4X))") "----", ("----------",M=1,3)

    do M = 2,50

        call MC_TRIAL(N,M,INTEG,ERR)
        write(*,"(I4,4X,3(F15.10,4X))") M, 1.0/sqrt(real(M)), INTEG, ERR

    end do

end program CORREL
```

Output:

```
 Result for 1 trial :   0.194797114

   M          1/SQRT(M)           INTEGRAL               ERROR
----         ----------         ----------          ----------
   2       0.7071067691       0.1974774301        0.0031326714
   3       0.5773502588       0.1930853277        0.0023623153
   4       0.5000000000       0.1938081384        0.0012355752
   5       0.4472135901       0.1949650347        0.0007936714
   6       0.4082482755       0.1954321414        0.0022544467
   7       0.3779644966       0.1909589916        0.0007706472
   8       0.3535533845       0.1933374107        0.0012095718
   9       0.3333333433       0.1901819408        0.0017845100
  10       0.3162277639       0.1929534823        0.0017424998
```

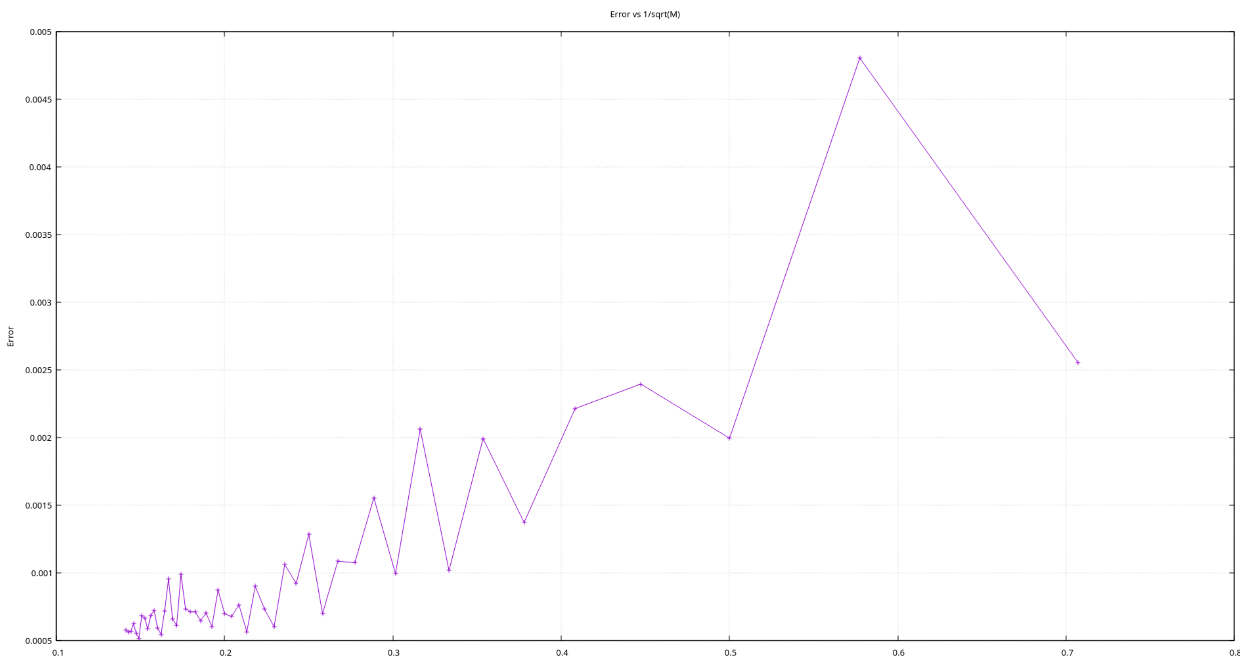

Figure 2: Error Analysis