

NSEG 5994 – Monte Carlo Methods for Particle Transport

Homework – 8

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The source codes for the two problems are provided at the end. Only the parts of the code that are modified for the calculation of scalar flux are provided.

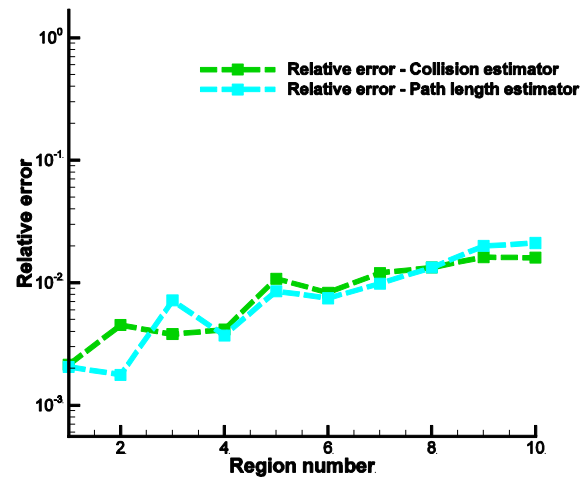
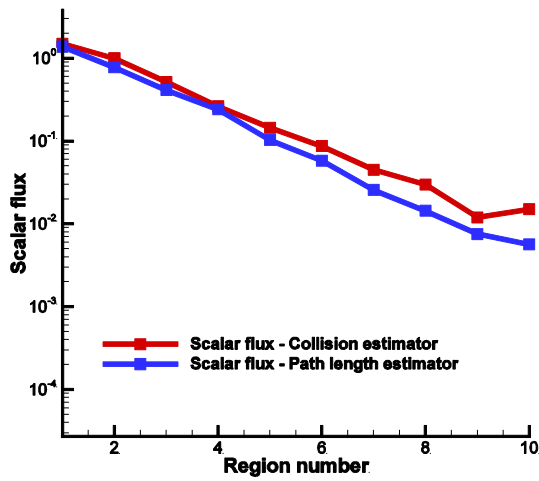
Problem 1:

The following tables provide results obtained from the analog code. The two cases – 10 and 50 regions used for the calculations are provided. For the second case, only the figure is provided. The following conclusions can be made from the results:

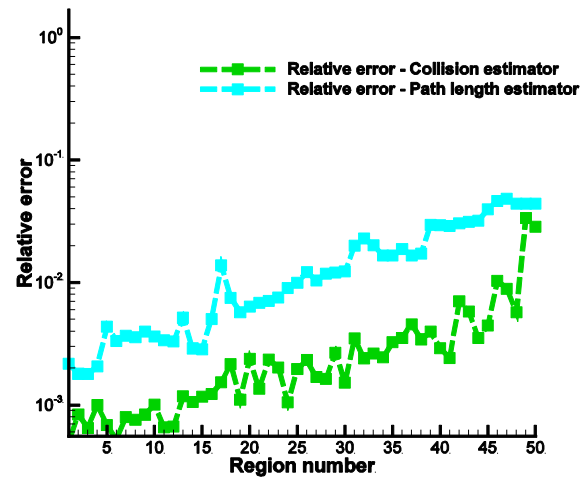
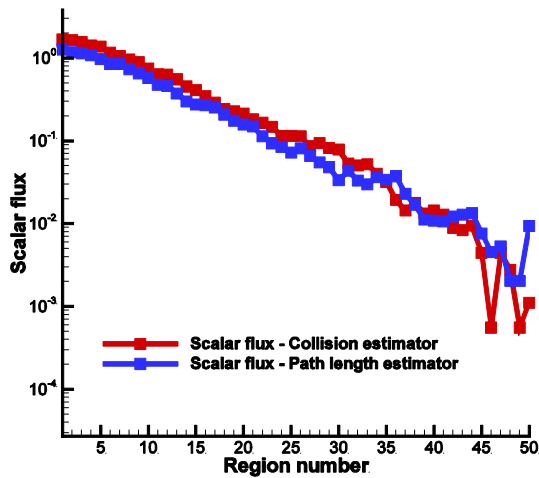
1. It is seen that as the distance from the source is increased, the scalar flux goes down.
2. The relative error on the other hand shows an increasing trend. This is probably due to the lower number of samples used for the scalar flux computation as the distance from the source increases.
3. Both the types of estimators provide similar estimates of scalar flux in most of the regions.

Number of regions – 10:

Region number	Collision estimator		Path length estimator	
	Scalar flux	Relative error	Scalar flux	Relative error
1	1.50E+00	2.15E-03	1.38E+00	2.06E-03
2	1.00E+00	4.51E-03	7.78E-01	1.77E-03
3	5.19E-01	3.81E-03	4.14E-01	7.18E-03
4	2.63E-01	4.15E-03	2.42E-01	3.71E-03
5	1.45E-01	1.08E-02	1.03E-01	8.53E-03
6	8.70E-02	8.29E-03	5.79E-02	7.47E-03
7	4.50E-02	1.20E-02	2.57E-02	9.84E-03
8	3.00E-02	1.33E-02	1.44E-02	1.33E-02
9	1.20E-02	1.62E-02	7.55E-03	2.00E-02
10	1.50E-02	1.60E-02	5.65E-03	2.11E-02



Number of regions – 50:



Problem 2:

Results are provided similar to the analog case.

The following conclusions can be made regarding the results obtained for geometric splitting case in comparison to the analog code results provided in the previous problem.

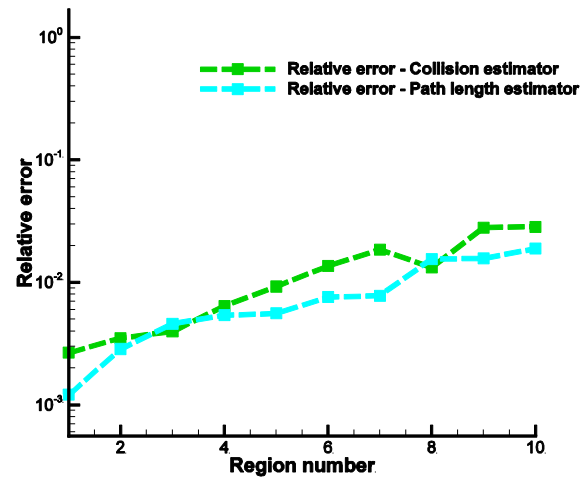
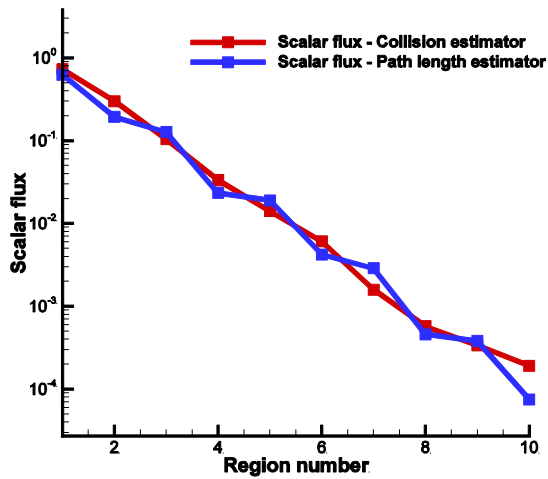
1. The scalar flux values obtained show a decreasing trend as the region under consideration is farther away from the source when 10 regions are considered. This is similar to the analog case. Though the trend appears the same, the values are to be noted here. The scalar flux itself

towards to the end of the detector has much lower values (almost 1-2 orders) than the predictions of the analog method.

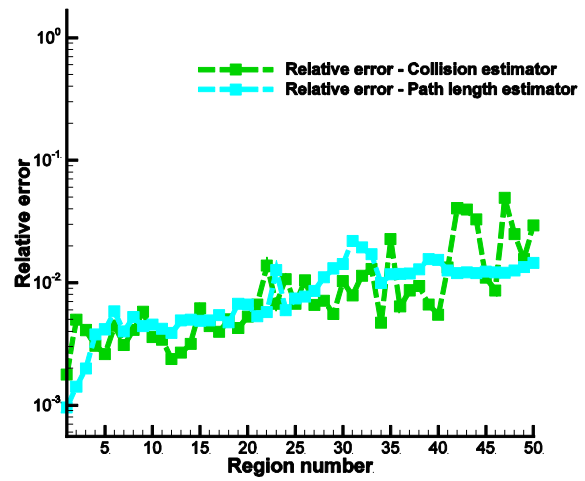
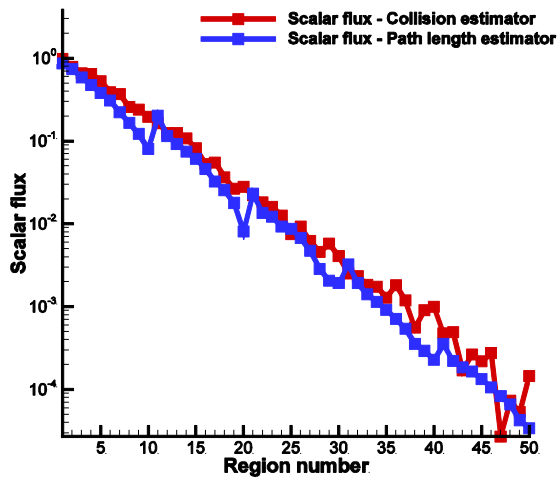
2. The relative errors obtained however, are slightly higher compared to the analog case throughout the domain. This can be related to the variance reduction technique that is applied. Since higher importance was provided for regions closer to the detector, more samples from those regions have been obtained in the calculation resulting in lesser number of samples in regions closer to the source. Hence, the higher errors in regions closer to the source.

Number of regions – 10:

Region number	Collision estimator		Path length estimator	
	Scalar flux	Relative error	Scalar flux	Relative error
1	7.28E-01	2.67E-03	6.23E-01	1.21E-03
2	2.99E-01	3.51E-03	1.94E-01	2.86E-03
3	1.04E-01	3.97E-03	1.27E-01	4.60E-03
4	3.33E-02	6.42E-03	2.34E-02	5.39E-03
5	1.41E-02	9.24E-03	1.90E-02	5.59E-03
6	6.07E-03	1.36E-02	4.22E-03	7.59E-03
7	1.59E-03	1.85E-02	2.88E-03	7.77E-03
8	5.74E-04	1.32E-02	4.58E-04	1.55E-02
9	3.39E-04	2.80E-02	3.82E-04	1.57E-02
10	1.92E-04	2.84E-02	7.52E-05	1.89E-02



Number of regions – 50:



Source code:

Problem 1 code:

```

MODULE allData

  TYPE shield
    REAL :: sigmaTotal, sigmaAbs, xMin, xMax, absRatio, thickness
  END TYPE shield

  TYPE (shield), ALLOCATABLE :: shld(:)

  INTEGER :: nParticles, nShields, parStatus, nParAbs, nParRef, &
    nParLeak, currentRegion, collStatus, freeFlightFlag, &
    nTallyingRegions
  REAL :: xInit, scatterAngleInit(3), xLocation, scatterAngle
  REAL :: probAbs(3), probRef(3), probLeak(3), &
    relativeErrorLeak(3), relativeErrorRef(3), &
    relativeErrorAbs(3), FOMLeak(3), FOMRef(3), FOMAbs(3), &
    varianceLeak(3), varianceRef(3), varianceAbs(3), &
    totalThickness
  REAL, ALLOCATABLE :: p(:), fc(:), scalarFluxColl(:), &
    scalarFluxPL(:), regionWidth(:), regionxMin(:), &
    regionxMax(:), scalarFluxCollSq(:), scalarFluxPLSq(:), &
    scalarFluxCollSum(:), &
    scalarFluxPLSum(:), relErrScalFlxColl(:), relErrScalFlxPL(:)

END MODULE allData

PROGRAM multiRegionShield

  USE allData

  IMPLICIT NONE

  INTEGER :: iParticle, iShield, unitProbFile, iScatterAngle, i, &
    n
  REAL :: pi, maxRelativeError, timeIn, timeOut, totalTime
  CHARACTER(80) :: nameProbFile

  ! Initialization
  xInit = 0.0
  pi = DACOS(-1.0)

```

```

CALL RANDOM_SEED()

nShields = 1
ALLOCATE(shld(nShields))

nTallyingRegions = 10
ALLOCATE(p(nTallyingRegions), fc(nTallyingRegions),      &
        scalarFluxColl(nTallyingRegions),                &
        scalarFluxPL(nTallyingRegions), regionxMin(nTallyingRegions), &
        regionxMax(nTallyingRegions), regionWidth(nTallyingRegions), &
        scalarFluxCollSq(nTallyingRegions),              &
        scalarFluxPLSq(nTallyingRegions),                &
        scalarFluxCollSum(nTallyingRegions),             &
        scalarFluxPLSum(nTallyingRegions),               &
        relErrScalFlxColl(nTallyingRegions),             &
        relErrScalFlxPL(nTallyingRegions))

shld(1)%thickness = 1.0
shld(1)%xMin = xInit
shld(1)%xMax = shld(1)%xMin + shld(1)%thickness
DO i = 1, nTallyingRegions
    regionxMin(i) = shld(1)%xMin + (i-1)*1.0/nTallyingRegions
    regionxMax(i) = shld(1)%xMin + i*1.0/nTallyingRegions
    regionWidth(i) = regionxMax(i) - regionxMin(i)
END DO
totalThickness = 0.0
DO n = 1, nShields
    totalThickness = totalThickness + shld(n)%thickness
END DO

shld(1)%sigmaTotal = 10.0
! shld(1)%sigmaAbs = 8.0 ! for ratio Es/Et = 0.2
shld(1)%sigmaAbs = 2.0 ! for ratio Es/Et = 0.8
shld(1)%absRatio = shld(1)%sigmaAbs/shld(1)%sigmaTotal

scatterAngleInit(1) = DCOS(0.0)
scatterAngleInit(2) = DCOS(pi/6.0)
scatterAngleInit(3) = DCOS(pi/3.0)
PRINT*, scatterAngleInit(:)

nParticles = 10000000

! Loop over the three scattering angles
DO iScatterAngle = 1, 1

    nParLeak = 0
    nParAbs = 0
    nParRef = 0
    maxRelativeError = 100.0

    iParticle = 0

    CALL CPU_TIME(timeIn)

    DO WHILE ((iParticle .LT. nParticles) .AND.      &
        (maxRelativeError .GT. 0.1))
        ! (maxRelativeError .GT. 0.0))

        iParticle = iParticle + 1
        IF (MOD(iParticle,1000000) .EQ. 0)          &
            PRINT*, 'particle number:', iParticle

        ! Initial x and mu values
        xLocation = xInit
        scatterAngle = scatterAngleInit(iScatterAngle)
        parStatus = 0
        currentRegion = 1
        collStatus = 0

        DO WHILE (parStatus .EQ. 0)

```

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CALL freeFlightPL

IF (parStatus .EQ. 0 .AND. collStatus .EQ. 1) &
    CALL getInteraction

IF (parStatus .EQ. 0 .AND. collStatus .EQ. 1) &
    CALL getScatterAngle

END DO

DO i = 1, nTallyingRegions
    scalarFluxColl(i) = fc(i)/iParticle/regionWidth(i)
    scalarFluxCollSq(i) = scalarFluxCollSq(i) &
        + scalarFluxColl(i)**2.0
    scalarFluxCollSum(i) = scalarFluxCollSum(i) &
        + scalarFluxColl(i)
    scalarFluxPL(i) = p(i)/iParticle/regionWidth(i)
    scalarFluxPLSq(i) = scalarFluxPLSq(i) + scalarFluxPL(i)**2.0
    scalarFluxPLSum(i) = scalarFluxPLSum(i) + scalarFluxPL(i)

    IF (MOD(iParticle,1000) .EQ. 0) THEN
        relErrScalFlxColl(i) = DSQRT((scalarFluxCollSq(i) &
            / (scalarFluxCollSum(i)**2.0)) - 1.0/iParticle)
        relErrScalFlxPL(i) = DSQRT((scalarFluxPLSq(i) &
            / (scalarFluxPLSum(i)**2.0)) - 1.0/iParticle)
        ! Following for collision estimator relative error
        IF (MINVAL(scalarFluxColl) .NE. 0.0) THEN
            maxRelativeError = MAXVAL(relErrScalFlxColl)
        END IF
        ! Following for path-length estimator relative error
        IF (MINVAL(scalarFluxPL) .NE. 0.0) THEN
            maxRelativeError = MAXVAL(relErrScalFlxPL)
        END IF
    END IF

END DO

END DO

CALL CPU_TIME(timeOut)
totalTime = timeOut - timeIn
totalTime = totalTime/60.0 ! Conversion to minutes

END DO

unitProbFile = 102
nameProbFile = 'problem_1b.dat'

OPEN (UNIT = unitProbFile, FILE = nameProbFile, &
    POSITION = 'append', FORM = 'formatted', ACTION = 'write')
DO i = 1, nTallyingRegions
    WRITE(unitProbFile,502) i, scalarFluxColl(i), &
        relErrScalFlxColl(i), &
        1.0/relErrScalFlxColl(i)**2./totalTime, &
        scalarFluxPL(i), relErrScalFlxPL(i), &
        1.0/relErrScalFlxPL(i)**2./totalTime
END DO
CLOSE(unitProbFile)

501 FORMAT (1(i1.1, 1X), 12(e12.5, 1X))
502 FORMAT (1(i2.2, 1X), 6(e12.5, 1X))

END PROGRAM multiRegionShield

SUBROUTINE freeFlightPL

USE allData

IMPLICIT NONE

INTEGER :: i, iOld, iNew

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REAL :: randNum, pathLength, regionPathLength, oldxLocation

CALL RANDOM_NUMBER(randNum)

pathLength = -LOG(randNum)/shld(currentRegion)%sigmaTotal
oldxLocation = xLocation
xLocation = xLocation + pathLength*scatterAngle

IF ((xLocation .GT. shld(currentRegion)%xMax)) THEN
  xLocation = shld(currentRegion)%xMax
  currentRegion = currentRegion + 1
  IF (currentRegion .GT. nShields) THEN
    parStatus = 1
    nParLeak = nParLeak + 1
  END IF
ELSE IF (xLocation .LT. shld(currentRegion)%xMin) THEN
  xLocation = shld(currentRegion)%xMin
  currentRegion = currentRegion - 1
  IF (currentRegion .LT. 1) THEN
    parStatus = 2
    nParRef = nParRef + 1
  END IF
ELSE
  collStatus = 1
! Collision estimator
  i = INT((xLocation-shld(1)%xMin) &
    *nTallyingRegions/totalThickness) + 1
  fc(i) = fc(i) + 1.0/shld(1)%sigmaTotal
END IF

iOld = INT((oldxLocation-shld(1)%xMin) &
  *nTallyingRegions/totalThickness) + 1
iNew = INT((xLocation-shld(1)%xMin) &
  *nTallyingRegions/totalThickness) + 1
IF (xLocation .EQ. 1.0) THEN
!   print*, iNew, xLocation, iOld
  iNew = nTallyingRegions
END IF

DO i = iOld, iNew
  IF (xLocation .GT. regionxMax(i)) THEN
    regionPathLength = (regionxMax(i)-oldxLocation)/scatterAngle
    p(i) = p(i) + 1.0*regionPathLength
    oldxLocation = regionxMax(i)
  ELSE
    regionPathLength = (xLocation-oldxLocation)/scatterAngle
    p(i) = p(i) + 1.0*regionPathLength
  END IF
END DO

! Path-length estimator

END SUBROUTINE freeFlightPL

```

Problem 2 code:

```

MODULE allData

  TYPE shield
    REAL :: sigmaTotal, sigmaAbs, xMin, xMax, absRatio, thickness, &
      importance
  END TYPE shield

  TYPE (shield), ALLOCATABLE :: shld(:, :)

  TYPE particle
    INTEGER :: region, subRegion
    REAL :: scatAngle, xLoc, weight
  END TYPE particle

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    TYPE (particle), POINTER :: next
END TYPE particle

TYPE (particle), POINTER :: parList, parListTail

INTEGER :: nParticles, nShields, parStatus, nParAbs, nParRef,      &
    nParLeak, currentRegion, collStatus, freeFlightFlag,          &
    nSubRegions, currentSubRegion, oldRegion, oldSubRegion,        &
    nTallyingRegions
REAL :: xInit, scatterAngleInit(3), xLocation, scatterAngle,      &
    parRef, parLeak, parAbs, parWeight, weightCutoff, parKilled,   &
    parAdded, impRatio
REAL :: probAbs(3), probRef(3), probLeak(3),                      &
    relativeErrorLeak(3), relativeErrorRef(3),                   &
    relativeErrorAbs(3), FOMLeak(3), FOMRef(3), FOMAbs(3),        &
    varianceLeak(3), varianceRef(3), varianceAbs(3),              &
    totalThickness
REAL, ALLOCATABLE :: p(:), fc(:), scalarFluxColl(:),              &
    scalarFluxPL(:), regionWidth(:), regionxMin(:),               &
    regionxMax(:), scalarFluxCollSq(:), scalarFluxPLSq(:),        &
    scalarFluxCollSum(:),                                          &
    scalarFluxPLSum(:), relErrScalFlxColl(:), relErrScalFlxPL(:)

END MODULE allData

PROGRAM multiRegionShield

USE allData

IMPLICIT NONE

INTEGER :: iParticle, iShield, unitProbFile, iScatterAngle,      &
    rrd, flag, numParLeft, iSubRegion, i, n
REAL :: pi, probLeakSq, probRefSq, probAbsSq, timeIn, timeOut,    &
    totalTime, maxRelativeError, iParLeak, iParRef, iParAbs
CHARACTER(80) :: nameProbFile

TYPE (particle), POINTER :: parCurrent, parTemp

INTERFACE

    SUBROUTINE insertPar(parCurrent,wt)

    USE allData
    TYPE (particle), POINTER, INTENT(IN) :: parCurrent
    REAL, INTENT (IN) :: wt

    END SUBROUTINE insertPar

END INTERFACE

! Initialization
xInit = 0.0
pi = DACOS(-1.0)
relativeErrorLeak = 100.0
relativeErrorAbs = 100.0
relativeErrorRef = 100.0

CALL RANDOM_SEED()

nShields = 1
nSubRegions = 5
impRatio = 3.4
ALLOCATE(shld(nShields,nSubRegions))

nTallyingRegions = 50
ALLOCATE(p(nTallyingRegions), fc(nTallyingRegions),              &
    scalarFluxColl(nTallyingRegions),                             &
    scalarFluxPL(nTallyingRegions),regionxMin(nTallyingRegions),  &
    regionxMax(nTallyingRegions), regionWidth(nTallyingRegions), &

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        scalarFluxCollSq(nTallyingRegions),      &
        scalarFluxPLSq(nTallyingRegions),        &
        scalarFluxCollSum(nTallyingRegions),      &
        scalarFluxPLSum(nTallyingRegions),        &
        relErrScalFlxColl(nTallyingRegions),      &
        relErrScalFlxPL(nTallyingRegions))

ALLOCATE(parList)
NULLIFY(parList%next)

DO iSubRegion = 1, nSubRegions
    shld(1,iSubRegion)%thickness = 1.0/nSubRegions
    shld(1,iSubRegion)%xMin = xInit + (iSubRegion-1)*1.0/nSubRegions
    shld(1,iSubRegion)%xMax = xInit + iSubRegion*1.0/nSubRegions

    shld(1,iSubRegion)%sigmaTotal = 10.0
    shld(1,iSubRegion)%sigmaAbs = 8.0 ! for ratio Es/Et = 0.2
!   shld(1,iSubRegion)%sigmaAbs = 2.0 ! for ratio Es/Et = 0.8
    shld(1,iSubRegion)%absRatio = &
        shld(1,iSubRegion)%sigmaAbs/shld(1,iSubRegion)%sigmaTotal

    shld(1,iSubRegion)%importance = impRatio**(iSubRegion-1.0)

END DO
DO i = 1, nTallyingRegions
    regionxMin(i) = shld(1,1)%xMin + (i-1)*1.0/nTallyingRegions
    regionxMax(i) = shld(1,1)%xMin + i*1.0/nTallyingRegions
    regionWidth(i) = regionxMax(i) - regionxMin(i)
END DO
totalThickness = 0.0
DO n = 1, nShields
    DO iSubRegion = 1, nSubRegions
        totalThickness = totalThickness + shld(n,iSubRegion)%thickness
    END DO
END DO

scatterAngleInit(1) = DCOS(0.0)
scatterAngleInit(2) = DCOS(pi/6.0)
scatterAngleInit(3) = DCOS(pi/3.0)

rrd = 5
weightCutoff = 1.0E-7
nParticles = 20000000

! Loop over the three scattering angles
DO iScatterAngle = 1, 3

    nParLeak = 0
    nParAbs = 0
    nParRef = 0
    parLeak = 0.0
    parRef = 0.0
    parAbs = 0.0
    parKilled = 0.0
    parAdded = 0.0
    probLeakSq = 0.0; probRefSq = 0.0; probAbsSq = 0.0
    maxRelativeError = 100.0

    iParticle = 0

    CALL CPU_TIME(timeIn)

    DO WHILE ((iParticle .LT. nParticles) .AND. &
        (maxRelativeError .GT. 0.1))

        iParticle = iParticle + 1
        IF (MOD(iParticle,100000) .EQ. 0) THEN
            PRINT*, 'particle number:', iParticle
        END IF

        xLocation = xInit

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scatterAngle = scatterAngleInit(iScatterAngle)
currentRegion = 1
currentSubRegion = 1
oldRegion = 1
oldSubRegion = 1
parWeight = 1.0
iParLeak = 0.0; iParRef = 0.0; iParAbs = 0.0
parListTail => parList
parCurrent => parListTail
CALL insertPar(parCurrent,parWeight)
parListTail => parCurrent%next
parCurrent => parCurrent%next

DO WHILE (ASSOCIATED(parCurrent))
  parStatus = 0
  currentRegion = parCurrent%region
  currentSubRegion = parCurrent%SubRegion
  oldRegion = currentRegion
  oldSubRegion = currentSubRegion
  collStatus = 0
  parWeight = parCurrent%weight
  xLocation = parCurrent%xLoc
  scatterAngle = parCurrent%scatAngle
  DO WHILE (parStatus .EQ. 0)

    CALL freeFlightPL

    IF (parStatus .EQ. 0 .AND. collStatus .EQ. 1) THEN
      CALL getInteraction
    END IF

    IF (parStatus .EQ. 0 .AND. collStatus .EQ. 1) THEN
      CALL getScatterAngle
    END IF

  END DO
  parCurrent => parCurrent%next
END DO

DO i = 1, nTallyingRegions
  scalarFluxColl(i) = fc(i)/iParticle/regionWidth(i)
  scalarFluxCollSq(i) = scalarFluxCollSq(i) &
    + scalarFluxColl(i)**2.0
  scalarFluxCollSum(i) = scalarFluxCollSum(i) &
    + scalarFluxColl(i)
  scalarFluxPL(i) = p(i)/iParticle/regionWidth(i)
  scalarFluxPLSq(i) = scalarFluxPLSq(i) + scalarFluxPL(i)**2.0
  scalarFluxPLSum(i) = scalarFluxPLSum(i) + scalarFluxPL(i)
  IF (MOD(iParticle,1000) .EQ. 0) THEN

    relErrScalFlxColl(i) = DSQRT((scalarFluxCollSq(i) &
      / (scalarFluxCollSum(i)**2.0)) - 1.0/iParticle)
    relErrScalFlxPL(i) = DSQRT((scalarFluxPLSq(i) &
      / (scalarFluxPLSum(i)**2.0)) - 1.0/iParticle)

    ! Following for collision estimator relative error
    ! IF (MINVAL(scalarFluxColl) .NE. 0.0) THEN
    ! maxRelativeError = MAXVAL(relErrScalFlxColl)
    ! END IF
    ! Following for path-length estimator relative error
    ! IF (MINVAL(scalarFluxPL) .NE. 0.0) THEN
    ! maxRelativeError = MAXVAL(relErrScalFlxPL)
    ! END IF
    ! END IF

  END DO

  CALL delParList
END DO

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    CALL CPU_TIME(timeOut)
    totalTime = timeOut - timeIn
    totalTime = totalTime/60.0 ! Conversion to minutes

END DO

unitProbFile = 102
nameProbFile = 'problem_2b.dat'

OPEN (UNIT = unitProbFile, FILE = nameProbFile,
      POSITION = 'append', FORM = 'formatted', ACTION = 'write') &
DO i = 1, nTallyingRegions
    WRITE(unitProbFile,502) i, scalarFluxColl(i), &
    relErrScalFlxColl(i), scalarFluxPL(i), relErrScalFlxPL(i)
END DO
CLOSE(unitProbFile)

501 FORMAT (1(i1.1, 1X), 12(e12.5, 1X))
502 FORMAT (1(i2.2, 1X), 4(e12.5, 1X))

END PROGRAM multiRegionShield

SUBROUTINE freeFlightPL

    USE allData

    IMPLICIT NONE

    INTEGER :: i, iOld, iNew
    REAL :: randNum, pathLength, regionPathLength, oldxLocation

    CALL RANDOM_NUMBER(randNum)

    pathLength = -LOG(randNum) &
    /shld(currentRegion,currentSubRegion)%sigmaTotal
    oldxLocation = xLocation
    xLocation = xLocation + pathLength*scatterAngle

    IF ((xLocation .GT. shld(currentRegion,currentSubRegion)%xMax)) &
    THEN
        xLocation = shld(currentRegion,currentSubRegion)%xMax
        oldSubRegion = currentSubRegion
        currentSubRegion = currentSubRegion + 1
        IF (currentSubRegion .GT. nSubRegions) THEN
            currentSubRegion = 1
            oldRegion = currentRegion
            currentRegion = currentRegion + 1
            IF (currentRegion .GT. nShields) THEN
                parStatus = 1
                nParLeak = nParLeak + 1
                parLeak = parLeak + parWeight
            END IF
        END IF
        IF (parStatus .EQ. 0) CALL geometricSplit
    ELSE IF (xLocation .LT. &
    shld(currentRegion,currentSubRegion)%xMin) THEN
        xLocation = shld(currentRegion,currentSubRegion)%xMin
        oldSubRegion = currentSubRegion
        currentSubRegion = currentSubRegion - 1
        IF (currentSubRegion .LT. 1) THEN
            currentSubRegion = nSubRegions
            oldRegion = currentRegion
            currentRegion = currentRegion - 1
            IF (currentRegion .LT. 1) THEN
                parStatus = 2
                nParRef = nParRef + 1
                parRef = parRef + parWeight
            END IF
        END IF
        IF (parStatus .EQ. 0) CALL geometricSplit
    ELSE

```

```

        collStatus = 1
! Collision estimator
        i = INT((xLocation-shld(1,1)%xMin)
                *nTallyingRegions/totalThickness) + 1
        fc(i) = fc(i) + parWeight/shld(1,1)%sigmaTotal

!   print*, 'collision'
END IF

iOld = INT((oldxLocation-shld(1,1)%xMin)
          *nTallyingRegions/totalThickness) + 1
iNew = INT((xLocation-shld(1,1)%xMin)
          *nTallyingRegions/totalThickness) + 1
IF (xLocation .EQ. 1.0) THEN
    print*, iNew, xLocation, iOld
    iNew = 10
END IF

DO i = iOld, iNew
    IF (xLocation .GT. regionxMax(i)) THEN
        regionPathLength = (regionxMax(i)-oldxLocation)/scatterAngle
        p(i) = p(i) + parWeight*regionPathLength
        oldxLocation = regionxMax(i)
    ELSE
        regionPathLength = (xLocation-oldxLocation)/scatterAngle
        p(i) = p(i) + parWeight*regionPathLength
    END IF
END DO

! Path-length estimator

END SUBROUTINE freeFlightPL

```