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Solution of Large Underestimation Problem in the Monte Carlo Calculation with Hard Biasing

-In Case with Geometry Input Data Created by CAD/MCNP Automatic Converter-

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An inconvenient experience was encountered, in which we have different answers depending on applied weight window values, in the nuclear analysis of the benchmark problem for CAD/MCNP interface programs, being developed under the ITER R&D task. Biasing can enhance calculation speed, but should not give different answers. Mechanism of this large underestimation is clarified. It is caused by the combination of the following two facts;

* When one of particles in a history has got lost, MCNP cancels all tallies calculated during the history and all banked particles are thrown away (never tracked).

* When we have distributed micro geometry errors in input data, important histories, which give significant contribution to tallies, will have many splitting and have "lost particle" with higher probability in the case of hard biasing.

These two facts lead to selective canceling of important histories. An attempt to eliminate this inconvenience has been made, by modifying the subroutine "hstory" of MCNP. The modification has been done very successfully and eliminated the large underestimation, giving the same answer independently from applied weight window values.

Keywords: Monte Carlo Code, MCNP, Hard Biasing, Weight Window, Large Underestimation, Lost Particles

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ITER の R&D タスクとして行なっている「CAD/MCNP 自動変換コードの開発」において、ベンチマ ーク問題の解析中、適用「weight window」の違いによって MCNP が異なる答えを出すという不都 合な事例に遭遇した.「weight window」法を含む"biasing"は計算速度を上げることがあっても、 異なる答えを出す様なことがあってはならない.本研究では、この「大きな過小評価」が起こる メカニズムを明らかにしプログラムの修正を行ったので報告する.「大きな過小評価」は、以下の 2つの事実の組合せでおこる:

- * MCNP はあるヒストリーの演算中に"lost particle"を検出すると当該ヒストリー中に計算 された全てのタリーをキャンセルしてしまう.また,その時点で splitting 等の結果バンクに 蓄積されていた粒子はその後追跡されることはない.
- * 微小形状エラーが入力に存在するとき,強バイアスの場合, "lost particle"を生じる確率 はヒストリーの重要度に大きく左右される.
- この結果, MCNP は選択的に重要度の高いヒストリーをキャンセルする事になる.

上記問題の解決を図るため, MCNP のサブルーチンのひとつである"hstory"の修正を行なった. テスト計算の結果, プログラムの修正は適切に行なわれ, MCNP は適用「weight window」に左右 されず同じ答えを出すようになったことが確認された.

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1. Introduction

Monte Carlo codes, such as MCNP [1,2], are powerful tool for nuclear analyses of devices with complicated geometry. When device size is very large and significant attenuation of radiation fluxes is expected, it is not easy to obtain results with good statistics even with using large supercomputers. In such cases we very often use biasing techniques, such as "weight windows". Those biasing can enhance calculation speed (can give smaller fractional standard deviation with the same number of histories or CPU time), but should not give different answers (mean values).

Because of severely limited space available for radiation shield in and around the torus, very high accuracy is required for nuclear analysis of ITER machine. In order to minimize estimation uncertainty in ITER device design calculation, most detailed and accurate geometry modeling is essential and development of CAD/MCNP interface program has been conducted under the ITER R&D task. Four parties (China, EU, Japan and USA) participate in this task and outcomes of their activities have been discussed periodically at the ITER task meetings.

In the course of analyzing the ITER benchmark problem defined in this task, we had an inconvenient experience in which different answers were obtained depending on applied weight window values. In this report we describe the problem we encountered (Chapter 2), causes of the problem (Chapter 3) and method to avoid such inconvenience (Chapter 4). Resolving the problem requires modification of one of the subroutines of MCNP program. The algorithm modification was made for MCNP5[1], although MCNP4C[2] was used in initial analysis of ITER CAD/MCNP benchmark problem. Those two versions showed the same behavior concerning with the present problem as shown in Appendix A.

2. Large underestimation encountered in the ITER CAD/MCNP benchmark neutron flux calculation

Figure 2.1 shows a 3-D CAD drawing of the ITER benchmark problem indicating four calculation tasks with MCNP. An inconvenience was observed in the calculation of the last one ④, which requires flux calculation in seven spheres located behind the port plug. Flux level behind the port plug is five orders of magnitude lower than that at the plasma region and most of neutrons which appear in the spaces behind the plug have reached there passing through the gaps between the plug and the port wall.

Comparison between Japanese and Chinese results [3] is shown in Fig. 2.2. Neutron fluxes in the plug region by the both parties agree very well, but those behind the plug have systematic difference between the both. Japanese calculation shows lower fluxes than Chinese one by a factor of about two. Neutron fluxes in the plug region and those in the gaps between the plug and port wall are shown in Fig. 2.3. This figure indicates that calculated fluxes in the plug by the both are similar but those in the gaps give quite different flux distributions.

By using MCNP plotting function, the gap geometries and surrounding material definitions were carefully compared between automatically converted geometry input data of the both parties. The both parties used their own CAD/MCNP conversion programs, namely MCAM [4] by China and GEOMIT [5] by Japan. However, no significant difference was found between the both geometry data.

In the following discussion, we mainly discuss about neutron fluxes in the first (closest to plasma) sphere ("#1 sphere" here after) out of the seven spheres behind the port plug in the equatorial port, since the difference between the both is systematic as shown in Fig. 2.2.

Figure 2.4 shows behaviors of the calculated fluxes in the #1 sphere by using the both input data changing width of weight windows (WUPN). There are two Japanese input data with different tables of weight windows (lower bound values); one is made for the target of photon flux in the sphere (ww1) and the other is for neutron flux in the sphere (ww2). In MCNP, lower bound of weight window of each cell is given as a table (WWN) and upper bound of the window is defined as WWN*WUPN, where WUPN value is separately given in a WWP card (default is WUPN=5). When we increase the width (WUPN), particles experience less splitting, becoming closer to non-biasing (analog) run. By observing this figure, one can imagine that Japanese calculations have some problem since their results change depending on the value of the weight window width and they agree with Chinese ones when the window width becomes sufficiently large. Especially from the fact, that Japanese calculation gives different neutron flux by just changing "mode" (neutron and photon calculation or that of neutron only), we are sure that something very inconvenient has happened in Japanese calculation.

Prominent difference in the input data by Japanese conversion code (GEOMIT) and by Chinese (MCAM) is that no lost particle is observed in the run with the latter input data while some lost particles with the former input data. Although the frequency is not high (about one lost particle per a ten thousand of histories), this is suspected to be a reason of the large underestimation in Japanese calculation with hard biasing. The explanation of the mechanism of this underestimation is given in the next chapter.

3. Mechanism of the large underestimation with hard biasing technique

3.1 Micro geometry errors in MCNP input data automatically converted from CAD files

Depending on maturity of interface programs developed in the four parties (China, EU, Japan and U.S.A), there exist "micro geometry errors" in input data automatically converted with them. An example found in the input data converted by the Japanese conversion program GEOMIT is shown in Fig. 3.1. The size of this example of error is very small (see Fig. 3.1 (e)). It is not easy to find this kind of error visually by using MCNP built-in plotting function but their locations can be found in the MCNP output list as a part of data concerning "lost particle". Because of the small error size, they usually do not affect calculation results, as far as hard biasing is not employed. However, they can give significant effect when hard biasing is used by the unique procedure of handling "lost particles" in MCNP. The next section explains this procedure.

3.2 The procedure of handling "lost particles" in MCNP

When a particle gets into "geometry error" like "undefined space", MCNP has a trouble in continuing tracing particle trajectory and clears all tallies calculated during random walks of all particles in this history (like Fig. 3.2 (b)), not only giving up its tracing and clearing tallies due to the specific "lost particle" (see Fig. 3.2 (a)). There still should be many particles in the bank in hard biasing cases when lost particle is detected, since splitting could have happened many times especially when this history provided particles in "very important locations (or cells)" for the calculation purpose of the present problem. Those particles banked during this history will be thrown away (never be traced, more exactly). Then, MCNP starts tracking the next history, without recording any tallies in this troubled history. This algorism can be confirmed by examining the subroutine "hstory" or conducting a simple test calculation which is shown in Appendix B.

This handling procedure of lost particles is not convenient for us when we have many scattered micro geometry errors in our input data. The probability with which the particle get into one of the micro errors can be proportional to the particle population. In hard biasing cases we make weight of particle very low and increase number of particles (or population) leading to high probability of "got lost", when it comes to important places (cells).

The combination of the above two facts leads to an inconvenient result of procedure, in which MCNP selectively cancels tallies of important histories, while it keeps all other histories as they are. This mechanism in hard biasing cases can lead to a large underestimation of calculation results.

4. Solution of the problem and modification of MCNP program

In order to solve the above problem, it is necessary to keep all histories in the calculation result without canceling their tallies even if lost particles are detected during random walks of those histories. Then MCNP may accept existence of micro geometry errors even in hard biasing cases. It can be a reasonable solution for this problem since it is not easy work to fully improve our CAD/MCNP automatic conversion program to completely eliminate micro geometry errors from its converted data.

In attempt of this solution, we slightly modified algorism of "hstory" in MCNP5 program. Actually, modification was made in the following two steps.

(1) First step modification : mod1

We inserted a few lines into the subroutine hstory program in order to

* avoid clearing calculated tallies during the present history, but

* go back to "bankit(100)" to take next particle stored in the bank

Continuation of tracking the "lost particle" itself is given up.

(2) Second steps : mod2-1 and mod2-2

In addition to the above (1), continuation of tracking the "lost particle" was made in two ways, slightly moving particle location forward in the flight direction of the present particle.

- * move back to the proper location in the program to continue tracking of the particle.(mod2-1)
- * stop tracking the present particle trajectory but bank a new particle which has the same weight, flight direction, energy, etc. as the lost particle, but slightly moved location forward. (mod2-2)

A list of lines modified in the subroutine "hstory.F90" is attached in Appendix C.

5. Test calculations

With using the modified subroutine "hstory", re-run of the ITER benchmark calculation has been conducted. Input data are the same as used in Fig. 2.2, which were automatically converted with GEOMIT from CAD data file. Test calculation results are shown in Fig.5.1, which compares neutron fluxes in #1 sphere by the MCNP with/without modified subroutine "hstory". All results with the modified subroutine, agree with Chinese result not depending on weight window and/or calculation mode (include photon calculation or not), while MCNP with original "hstory" gives very different answers depending on weight window and calculation mode. Since all three modifications give practically the same answer, tracking the "lost particle" itself looks not important, at least for the present problem. Concerning with Chinese input data, we have no "lost particle" and the same results were obtained by the both of original and modified MCNP versions.

Figure 5.2 shows dependence of weight window width on the neutron flux tested with using mod2-2 "hstory.F90" subroutine. Now we have the same answer independently from WUPN value as shown in this Fig. 5.2. Comparison with Chinese results is again shown in Figs. 5.3 and 5.4, replacing Japanese results with the new ones, which are obtained with modified MCNP5 (mod2-2). Fluxes in the gaps between port wall and the plug calculate by the both parties agreed very well, as well as those behind the port plug.

Figures 5.5 and 5.6 show similar comparison but with other participating countries; EU and USA[3]. From theses figures we can say that agreement of the results from all participating parties' CAD/MCNP interface programs on ④ task in Fig.2.1 has become rather well, leaving only 20 % difference among them.

6. Concluding remarks

The following conclusions have been obtained through the present study;

(1) Mechanism of large underestimation in cases of hard biasing was clarified. It is caused by the combination of the following two facts;

* MCNP cancels all tallies calculated during the history, when one of particles in the history gets lost.

* When we have distributed micro geometry errors, for example ITER 3-D model converted with our

CAD/MCNP interface program (GEOMIT) from CAD drawing, important histories will have "lost particle" with high probability in the case of hard biasing.

These facts lead to selective canceling of important histories.

(2) The attempt to eliminate the large underestimation in case of hard biasing has been made successfully, by modifying subroutine "hstory.F90" of MCNP5. Three modified versions of the "hstory.F90" have been produced and they give practically the same answer, which is judged to be reasonable.

(3) Comparison of the fluxes behind the port plug with other parties (CN, EU and USA) showed rather good agreement, indicating that the CAD/MCNP interface programs developed by all parties are approaching a matured level for using in real design analysis of the machines.

(4) All calculations of the ITER CAD/MCNP benchmark problem, conducted by MCNP4C were re-conducted by using MCNP5, and it is confirmed that the both version give same answers.

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References

- X-5 Monte Carlo Team, "MCNP A General Monte Carlo N-Particle Transport Code, Version 5", LA-UR-03-1987 (April 24, 2003: Revised 10/3/05)
- J.F. Briesmeister (ed.), "MCNP A General Monte Carlo N-Particle Transport Code, Version 4C", LA-13709-M, April 2000.
- [3] P. Wilson, et al., "State-of-the-art 3-D Neutronics Analysis Methods for Fusion Energy Systems", S2-0001, 8th International Symposium on Fusion Nuclear Technology, Heidelberg, Germany, October, 2007
- [4] Y. Wu, Y Li, L. Lu, et al., "Research and development of the automatic modeling system for Monte Carlo particle transport simulation", Chinese J. Nuclear Science & Engineering, 26 (1) pp. 20-27, (2006).
- [5] N. Aly, F. Masuda, H. Nasif, S. Sato, H. Iida, T. Nishitani, M. Yamada, H. Sawamura, H. Morota, "A New Developed Interface for CAD/MCNP Data Conversion", 14th International Conference on Nuclear Engineering, Miami, Florida, USA, July 17-20, 2006, ICONE 14-89742.



Fig. 2.1 CAD model of the ITER benchmark geometry and MCNP calculation tasks



Fig. 2.2 Comparison of neutron fluxes in and behind the port plug between Japanese and Chinese calculations (with MCNP4C):④ task shown in Fig. 2.1



Fig. 2.3 Comparison of neutron fluxes in the port plug (plug), those in the vertical gaps (vg) and horizontal gaps (hg) between Japanese and Chinese calculations (with MCNP4C)



Fig. 2.4 Effect of weight window width (WUPN) on the neutron flux at the #1 sphere behind the port plug (with MCNP4C)



Fig. 3.1 An example of micro geometry errors in the input data automatically converted with GEOMIT from CAD data file



Fig. 3.2 Schematic explanation of MCNP lost particle handling procedure



Fig. 5.1 Neutron fluxes in the #1 sphere behind the port plug of the ITER benchmark problem with modified subroutines "hstory.F90" (WUPN value: default of 5)



Fig. 5.2 Effect of weight window width (WUPN) on the neutron flux at the #1 sphere behind the port plug with modified MCNP5: (mod2-2)



Fig. 5.3 Comparison of neutron fluxes in and behind the port plug between Japanese (with modified MCNPv5: mod2-2) and Chinese calculations (④ task shown in Fig.2.1)



Fig. 5.4 Comparison of neutron fluxes in the plug(plug), those in the vertical gaps (vg) and horizontal gaps (hg) between Japanese (with the modified MCNP5:mod2-2) and Chinese calculations



Fig. 5.5 Comparison of neutron fluxes in and behind the port plug among all participating parties in the CAD/MCNP benchmark tasks (④ task shown in Fig.2.1)



Fig. 5.6 Comparison of neutron fluxes behind the plug among all participating parties in the CAD/MCNP benchmark tasks (④ task shown in Fig.2.1)

Appendix A Comparison of neutron fluxes behind the plug between MCNP4C and MCNP5

The underestimation problem was detected in calculations with MCNP4C and we modified MCNP5 program. Then, in order to assure that the both version of MCNP gives same results, comparative study has been done. The results are shown in Fig. A-1. It can be said that we have almost complete agreement between results of the both versions of MCNP.



Fig. A-1 Comparison of neutron fluxes behind the plug between those calculated with MCNP4C and MCNP5 (Chinese input data is employed))

Appendix B Test calculation for confirming "lost particle handling" in MCNP

In order to visually understand how MCNP behaves when it gets "lost particle", a test run has been made as shown in Fig.B-1. The calculation model is an empty box of $2m \times 2m \times 2m$, with a 2 cm thick thin region (from x=-1 to 1) of source cell. Source particles born homogenously in this region and travel in parallel with X axis (40% in - direction and other 60% in + direction).

At x=-50 a very thin region (1 mm) is located where calculation condition is changed as follows;

- (a) Case 1 : normal void region with importance=1
- (b) Case 2 : normal void region with importance=0, then particles are killed when they have reached here.
- (c) Case 3 : this region is "undefined region" in MCNP input data; namely "geometry error". When particles reach this region, they are got lost.

Test calculation results are shown in Fig.B-2. When the geometry is correctly produced (case 1) the result looks very reasonable and ratio of flux levels on x>0 side and x<0 side is 6 : 4 corresponding to emission rates of source particle in both directions. When importance in the thin region at x=-50 cm is set to be 0 (case 2), the flux at x < -50 cm become zero, but no change in other location. If we have geometry error (undefined region) at x= -50 cm, all fluxes at x < 0 become zero although particles should have been traced normally until reaching the thin region at x=-50 cm. This shows clearly that MCNP cancels all tallies it calculated during the present history.



Fig. B-1Test calculation model for examining how "lost particles" are treated in MCNP



Fig. B-2 Results of the test calculation for examining how "lost particles" are treated in MCNP

Appendix C Modified part of subroutine "hstory.F90" of MCNP5

The modified parts of the subroutine "hstory.F90" of MCNP5.1.40 are listed below for the cases of (1)mod1, (2)mod2-1 and (3)mod2-2.

```
(1) Modification of "hstory.F90" for mod1
```

541a542,543

> kdb = 0

> go to 260

```
(2) Modification of "hstory.F90" for mod2-1
1,3d0
<!+ $Id: hstory.F90,v 1.8.2.1 2005/10/04 22:46:16 jsweezy Exp $
< ! Copyright LANL/UC/DOE - see file COPYRIGHT_INFO
<
6a4
>
    !* hstory.F90.Low_ok *
15,17d12
< #if defined(VISED) && defined(DEC)
    use c_interfaces
<
< #endif
23a19,28
> !*Lower*B
    integer :: lgcwk(mlgc+1)
>
    integer :: ncel_pl(10)
>
    integer :: loop_ctr
>
> !*Lower*E
>
    integer
              jerr
                                    !*Debug*
    jerr=0
                                      !*Debug*
>
> !*Lower*B
    loop_ctr=0
>
> !*Lower*E
42a48,50
>! if(nps.eq.lost_num) then
                                               !*Debug*
>! write(6,*) 'hstory-R: Label_020',nps,icl !*Debug*
>! endif
                                                   !*Debug*
54c62,65
```

```
if( kdb/=0 ) go to 390
<
---
    if( kdb/=0 ) then
>
     jerr=1
                     !*Debug*
>
      go to 390
>
    endif
>
76c87,90
<
       if( kdb/=0 ) go to 390
---
       if( kdb/=0 ) then
>
>
        jerr=2
                        !*Debug*
>
         go to 390
       endif
>
94c108,111
    if( kdb/=0 ) go to 390
<
----
    if( kdb/=0 ) then
>
       jerr=3
                      !*Debug*
>
>
       go to 390
    endif
>
152c169,172
<
           if( kdb/=0 ) go to 390
---
          if(kdb/=0) then
>
             jerr=4
                            !*Debug*
>
             go to 390
>
           endif
>
231c251,254
    if( kdb/=0 ) go to 390
<
---
   if(kdb/=0) then
>
      jerr=5
                     !*Debug*
>
>
      go to 390
    endif
>
237c260,263
<
      if( kdb/=0 ) go to 390
---
>
      if( kdb/=0 ) then
```

```
!*Debug*
>
         jerr=6
>
         go to 390
>
       endif
335c361,364
      if( d==dls ) then
<
---
    if( d==dls ) then
>
> !*Lower*B
>
      jrtry=0
> !*Lower*E
340c369,469
       if( kdb/=0
<
                   ) go to 390
---
       if( kdb/=0
                   ) then
>
> !*Lower*B
>
         loop_ctr=loop_ctr+1
> !*Debug*B
> ! write(6,'(60hHSTORY-R: Aft_surfac,kdb/=0. nps,kdb,icl,jsu,loop_ctr,mynum=, &
> !& i8,i4,2i8,2i4)') nps,kdb,icl,jsu,loop_ctr,mynum
> !*Debug*E
>
         if(loop_ctr.gt.100) then
           jerr=71
                                     !*Debug*
>
>
           go to 390
         endif
>
>
         if(jrtry.eq.0) then
>
           x_{WW} = xxx
>
           y_ww=yyy
>
           z WW = zzz
>
           u_ww =uuu
>
           v_ww=vvv
>
           w_ww =www
>
           d_ww = d
>
           iclwk=icl
>
           jsuwk=jsu
           kdbw =kdb
>
         endif
>
>
```

```
> !* shift (x,y,z), find the unique 'icl'
```

```
> 110 continue
>
         jrtry=jrtry+1
>
         if(jrtry.gt.10) go to 120
         kdb = 0
>
         xxx=xxx+u ww*1.d+00
>
         yyy=yyy+v_ww*1.d+00
>
         zzz=zzz+w ww*1.d+00
>
>
         n_pl=0
>
         do i=1,mxa
            call chkcel(i,0,k)
>
>
            if(k.eq.0) then
>
              j2=abs(lca(i))
>
              j3=abs(lca(i+1))
              do j=1,j3-j2+1
>
                 lgcwk(j)=lgc(j)
>
>
              enddo
>
              n_pl=n_pl+1
              ncel_pl(n_pl)=i
>
              go to 112
>
            endif
>
>
         enddo
> 112 continue
         if(n_pl.ne.1) go to 110
                                  !*retry 'shift (x,y,z)'
>
>
         icl=ncel_pl(1)
         ic9=ic1
>
>
> !* change 'jsu'
>
         j2=abs(lca(ic9))
         j3=abs(lca(ic9+1))
>
         do j=1,j3-j2+1
>
            lgc(j)=lgcwk(j)
>
         enddo
>
>
         call track(ic9)
         if(kdb.ne.0) go to 110
                                   !*retry 'shift (x,y,z)'
>
>!
>
         uuu=-u ww
>
         vvv=-v_ww
>
         www=-w_ww
```

```
> do j=1,j3-j2+1
```

> lgc(j)=lgcwk(j)

```
> enddo
```

```
> call track(ic9)
```

```
> !*???*B
```

```
> if(kdb.ne.0) then
```

```
> uuu=u_ww
```

- > vvv=v_ww
- > www=w_ww
- > go to 110 !*retry 'shift (x,y,z)'

```
> endif
```

> ! write(6,*) 'HSTORY-R: go to the next cell process.'

>!*???*E

- > jsu=jap
- > uuu=u_ww
- > vvv=v_ww
- > www=w_ww
- > do j=1,j3-j2+1
- > lgc(j)=lgcwk(j)
- > enddo
- > d =d_ww
- > go to 50 !* go to the next cell process.
- >
- > 120 continue
- > kdb=kdbw
- > jsu=jsuwk
- > icl=iclwk
- > d =d_ww
- > uuu=u_ww
- > vvv=v_ww
- > www=w_ww
- > xxx=x_ww
- > yyy=y_ww
- > zzz=z_ww

```
> !*Lower*E
```

- > jerr=7 !*Debug*
- > go to 390
- > endif

```
380c509,512
<
    if( kdb = 0
                   ) go to 390
---
    if( kdb/=0
                    ) then
>
                       !*Debug*
      jerr=8
>
       go to 390
>
    endif
>
391c523,526
    if( kdb/=0 ) go to 390
<
---
    if( kdb/=0 ) then
>
      jerr=9
                       !*Debug*
>
>
       go to 390
>
    endif
396c531,534
       if( kdb/=0 ) go to 390
<
---
>
       if( kdb/=0 ) then
         jerr=10
                         !*Debug*
>
>
         go to 390
>
       endif
503a642
>
      jerr=11
                      !*Debug*
541a681,690
> !*Debug*B
    write(6,'(53hHSTORY-R: L390. jerr,nps,icl,kdb,loop ctr,mynum,nbnk=, &
>
> & i2,i10,i8,3i4,i8)') jerr,nps,icl,kdb,loop_ctr,mynum,nbnk
> !*Debug*E
> !
> !*Lower*B
>
      kdb=0
     loop_ctr=0
>
      go to 260
                    !* for unbanking.
>
> !*Lower*E
543d691
<
```

```
(3) Modification of "hstory.F90" for mod2-2
53a54
> if( kdb/=0
               ) ipath
                             =1
75a77
>
       if( kdb/=0
                     ) ipath
                                =2
93a96
> if( kdb/=0
               ) ipath
                             =3
151c154,155
           call forcol
<
---
>
           call forcol
           if( kdb/=0
>
                        ) ipath
                                   =4
230a235
> if( kdb/=0
               ) ipath
                             =5
236a242
>
      if( kdb/=0
                 ) ipath
                               =6
339a346
>
      if( kdb/=0
                   ) ipath
                               =7
379a387
> if( kdb/=0
                             =8
                 ) ipath
390a399
> if( kdb/=0 ) ipath
                             =9
395a405
>
      if( kdb/=0 ) ipath
                               =10
503a514
>
      ipath
               =11
541a553,636
>!
            write(iuo ,16) ipath ,kdb,npa,mxa
>!16
            format( "ipath = ", i6, "kdb= ",i6, "npa = ",i6,"mxa = ",i6)
>
    if( kdb<=0.or.kdb>=11 ) go to 580
>
    if( kdb==2 .or. kdb==4 .or. kdb==6 ) go to 580
    if( icl > mxa ) go to 580
>
    ! determine whether the particle really is in cell icl.
>
>
      uuu = -uuu
      vvv = -vvv
>
>
      www = -www
    call chkcel(icl,0,j1)
>
```

```
> if(j1/=0) then
```

```
>
       do iq = 1,mxa
>
         call chkcel(iq,0,j2)
>
         if(j2==0) exit
       enddo
>
       icl=iq
>
      endif
>
>
      uuu = -uuu
>
      vvv = -vvv
      www = -www
>
       do 261 iida=1,10
>
          aiida=iida
>
          dskip=rdum(5)/5*aiida
>
>!
            dskip=rdum(5)
           write(iuo ,14) xxx,yyy,zzz,uuu,vvv,www,icl,iii,jjj,kkk,nbnk
>!
>!14
            format( "yyy)", 6e12.5,5i6)
          xxx = xxx + uuu*dskip
>
>
          yyy = yyy + vvv*dskip
>
          zzz = zzz + www*dskip
       do iq = 1,mxa
>
         call chkcel(iq,0,j2)
>
         if(j2==0) exit
>
       enddo
>
>
       if( iq > mxa) cycle
       if( iq==icl ) cycle
>
>! function wwval(ny,nc,nb,na,ix)
>
        nb=1
        wwva=wwval(ipt,iq ,nb,0,0)
>
        if(wwva<0.0) then
>
>
          xxx = xxx - uuu*dskip
          yyy = yyy - vvv*dskip
>
>
          zzz = zzz - www*dskip
          go to 580
>
        endif
>
>
        iid=icl
>
        icl=iq
>
        iicl=ncl(icl)
        iiid=ncl(iid)
>
>
```

```
>!
        write(iuo,542) lev,iiid,icl,iicl,iida,ipt,wwva,rdum(5),dskip,erg,wgt
>! 542
            format("OK!",6i6,6e9.2)
> !
              write(iuo ,13) xxx,yyy,zzz,uuu,vvv,www,icl,iii,jjj,kkk
>!13
             format( "xxx)", 6e12.5,4i7)
          do j=0,lev
>
            udt(1, j) = xxx
>
>
            udt(2, j) = yyy
            udt(3, j) = zzz
>
            udt(4, j) = uuu
>
            udt(5, j) = vvv
>
>
            udt(6, j) = www
>
            udt(7, j) = icl
            udt(8, j) = iii
>
            udt(9, j) = jjj
>
            udt(10, j) = kkk
>
>
           end do
>!
               write(iuo ,11) iicl, iiid, lev, ji
>!11
             format("iicl,iiid,lev,ji,levchk", 5i6)
>!
              write(iuo,12) (udt(i,lev),i=1,10),nbnk,iida
>! 12
             format( "udt(1-10,lev)", 6e12.5,4f7.1,2i6)
>!
              kdb = 0
>!
              if( npa == 0 ) npa = 1
                                           !iida
            npa = 1
                           !iida
>
            if (ipt==1) call bankit(7)
>
            if (ipt==2) call bankit(8)
>
            kdb = 0
>
>!
             write(iuo ,15) nbnk
>!15
             format( "nbnk =", i6)
>
           go to 260
> 261
          continue
> 580 continue
         write(iuo,541) icl,iq,ncl(icl), xxx, yyy, zzz,kdb,wwva
>!
>! 541
            format("580 icl,iq x,y,z kdb wwva",3i6,3e12.5,i6,e9.2)
           kdb = 0
>
>
       go to 260
\sim
```

表1. SI 基本単位					
其木島	SI 基本)	単位			
巫平里	名称	記号			
長さ	メートル	m			
質 量	キログラム	kg			
時 間	秒	S			
電 流	アンペア	А			
熱力学温度	ケルビン	Κ			
物質量	モル	mol			
光 度	カンデラ	cd			

表2. 基本単位を用いて表されるSI組立	単位の例
----------------------	------

组去早	SI 基本単位			
和工生	名称	記号		
面 積	平方メートル	m ²		
体積	立法メートル	m ³		
速 さ , 速 度	メートル毎秒	m/s		
加 速 度	メートル毎秒毎秒	m/s^2		
波 数	毎メートル	m-1		
密度(質量密度)	キログラム毎立法メートル	kg/m^3		
質量体積(比体積)	立法メートル毎キログラム	m ³ /kg		
電流密度	アンペア毎平方メートル	A/m^2		
磁界の強さ	アンペア毎メートル	A/m		
(物質量の)濃度	モル毎立方メートル	$mo1/m^3$		
輝 度	カンデラ毎平方メートル	cd/m^2		
屈 折 率	(数の) 1	1		

表 5. SI 接頭語							
乗数	接頭語	記号	乗数	接頭語	記号		
10 ²⁴	Э 9	Y	10^{-1}	デシ	d		
10^{21}	ゼタ	Z	10^{-2}	センチ	с		
10^{18}	エクサ	Е	10^{-3}	ミリ	m		
10^{15}	ペタ	Р	10^{-6}	マイクロ	μ		
10^{12}	テラ	Т	10^{-9}	ナノ	n		
10^{9}	ギガ	G	10^{-12}	ピョ	р		
10^{6}	メガ	Μ	10^{-15}	フェムト	f		
10^{3}	キロ	k	10^{-18}	アト	а		
10^{2}	ヘクト	h	10^{-21}	ゼプト	Z		
10 ¹	デ カ	da	10^{-24}	ヨクト	у		

表3. 固有の名称とその独自の記号で表されるSI組立単位 組み用な

	51 租业单位			
組立量	名称	記号	他のSI単位による	SI基本単位による
			表し方 あんし	表し方
平 面 角	ラジアン ^(a)	rad		$m \cdot m^{-1} = 1^{(b)}$
立 体 角	ステラジアン ^(a)	$\mathrm{sr}^{(c)}$		$m^2 \cdot m^{-2} = 1^{(b)}$
周 波 数	ヘルツ	Hz		s ⁻¹
力	ニュートン	Ν		m•kg•s ⁻²
压力, 応力	パスカル	Pa	N/m^2	$m^{-1} \cdot kg \cdot s^{-2}$
エネルギー,仕事,熱量	ジュール	J	N•m	$m^2 \cdot kg \cdot s^{-2}$
工率,放射束	ワット	W	J/s	$m^2 \cdot kg \cdot s^{-3}$
電荷,電気量	クーロン	С		s•A
電位差(電圧),起電力	ボルト	V	W/A	$m^2 \cdot kg \cdot s^{-3} \cdot A^{-1}$
静電容量	ファラド	F	C/V	$m^{-2} \cdot kg^{-1} \cdot s^4 \cdot A^2$
電気抵抗	オーム	Ω	V/A	$m^2 \cdot kg \cdot s^{-3} \cdot A^{-2}$
コンダクタンス	ジーメンス	S	A/V	$m^{-2} \cdot kg^{-1} \cdot s^3 \cdot A^2$
磁東	ウェーバ	Wb	V•s	$m^2 \cdot kg \cdot s^{-2} \cdot A^{-1}$
磁束密度	テスラ	Т	Wb/m^2	$kg \cdot s^{-2} \cdot A^{-1}$
インダクタンス	ヘンリー	Н	Wb/A	$m^2 \cdot kg \cdot s^{-2} \cdot A^{-2}$
セルシウス温度	セルシウス度 ^(d)	°C		K
光東	ルーメン	1m	$cd \cdot sr^{(c)}$	$m^2 \cdot m^{-2} \cdot cd = cd$
照度	ルクス	1x	1m/m^2	$m^2 \cdot m^{-4} \cdot cd = m^{-2} \cdot cd$
(放射性核種の) 放射能	ベクレル	Bq		s ⁻¹
吸収線量, 質量エネル	H L I	Cu	T /lr.m	22
ギー分与, カーマ		чу	J/Kg	m•s
線量当量,周辺線量当		_	- 4	
量,方向性線量当量,個	シーベルト	Sv	J/kg	$m^2 \cdot s^{-2}$
人線重当重,組織線重当				L

(a) ラジアン及びステラジアンの使用は、同じ次元であっても異なった性質をもった量を区別するときの組立単位の表し方として利点がある。組立単位を形作るときのいくつかの用例は表4に示されている。
 (b) 実際には、使用する時には記号rad及びsrが用いられるが、習慣として組立単位としての記号"1"は明示されない。
 (c) 測光学では、ステラジアンの各称と記号srを単位の表し方の中にそのまま維持している。

(d)この単位は、例としてミリセルシウス度m℃のようにSI接頭語を伴って用いても良い。

表4. 単位の中に固有の名称とその独自の記号を含むSI組立単位の例

如去县	SI 組立単位			
和立里	名称	記号	SI 基本単位による表し方	
粘	度パスカル秒	Pa•s	$m^{-1} \cdot kg \cdot s^{-1}$	
力のモーメン	トニュートンメートル	N • m	$m^2 \cdot kg \cdot s^{-2}$	
表 面 張	力ニュートン毎メートル	N/m	kg • s ⁻²	
角速	度ラジアン毎秒	rad/s	$m \cdot m^{-1} \cdot s^{-1} = s^{-1}$	
角 加 速	度ラジアン毎平方秒	rad/s^2	$m \cdot m^{-1} \cdot s^{-2} = s^{-2}$	
熱流密度,放射照	度 ワット毎平方メートル	W/m^2	$kg \cdot s^{-3}$	
熱容量,エントロピ	ージュール毎ケルビン	J/K	$m^2 \cdot kg \cdot s^{-2} \cdot K^{-1}$	
質量熱容量 (比熱容量)	, ジュール毎キログラム	$I/(k \sigma \cdot K)$	-22 - V ⁻¹	
質量エントロピ	ー 毎ケルビン	J/ (kg · k)	m·s·k	
質量エネルギ	ージュール毎キログラム	I/ka	$m^2 \cdot a^{-2} \cdot k^{-1}$	
(比エネルギー)	J/ Kg	m · s · k	
執 伝 道	マット毎メートル毎ケ	W/(m•K)	$m \cdot k \sigma \cdot c^{-3} \cdot K^{-1}$	
	「ルビン	117 (m 117)	m Kg S K	
休積エネルギ	_ ジュール毎立方メート	T/m^3	$m^{-1} \cdot k \sigma \cdot s^{-2}$	
	N	J7 m	m ng 5	
電界の強	さボルト毎メートル	V/m	$\mathbf{m} \cdot \mathbf{kg} \cdot \mathbf{s}^{-3} \cdot \mathbf{A}^{-1}$	
体 積 雷	荷クーロン毎立方メート	C/m^3	m ⁻³ • s • A	
		07 11	in o n	
電 気 変	位クーロン毎平方メート	C/m^2	m ⁻² • s • A	
			-2 -1 4 2	
誘 電	率ファフド毎メートル	F/m	$m^3 \cdot kg^1 \cdot s^* \cdot A^2$	
透 燃	率ヘンリー毎メートル	H/m	$m \cdot kg \cdot s^2 \cdot A^2$	
モルエネルキ	ーシュール毎モル	J/mol	m • kg • s [°] • mol '	
モルエントロビー	, ジュール毎モル毎ケル	J/(mol • K)	$m^2 \cdot kg \cdot s^{-2} \cdot K^{-1} \cdot mol^{-1}$	
モル熱谷		a /1	1	
照射線重 (X線及びγ線	ノ クーロン毎キロクフム	C/kg	kg [•] •s•A	
败 収 禄 重	半クレイ 母 秒	Gy/S	m ⁻ •s ⁻ 4 -2 , -3 2 , -3	
<i>I</i> 队	度 ワットサイアフンノン	W/sr	m [*] •m [*] •kg•s [°] =m [*] •kg•s [°]	
放 射 輝	度気をするション	$W/(m^2 \cdot sr)$	$m^2 \cdot m^{-2} \cdot kg \cdot s^{-3} = kg \cdot s^{-3}$	

表6. 国際単位系と併用されるが国際単位系に属さない単位

名称	記号	SI 単位による値
分	min	1 min=60s
時	h	1h =60 min=3600 s
日	d	1 d=24 h=86400 s
度	0	$1^{\circ} = (\pi / 180)$ rad
分	,	1' = $(1/60)^{\circ}$ = $(\pi/10800)$ rad
秒	"	1" = $(1/60)$ ' = $(\pi/648000)$ rad
リットル	1, L	$11=1 \text{ dm}^3=10^{-3}\text{m}^3$
トン	t	1t=10 ³ kg
ネーパ	Np	1Np=1
ベル	В	$1B=(1/2)\ln 10$ (Np)

表7. 国際単位系と併用されこれに属さない単位で SI単位で表される数値が実験的に得られるもの					
名称	記号	SI 単位であらわされる数値			
電子ボルト	eV	$1 \text{eV}=1.60217733(49) \times 10^{-19} \text{J}$			
統一原子質量単位	u	1u=1.6605402(10)×10 ⁻²⁷ kg			
天 文 単 位	ua	1ua=1.49597870691(30)×10 ¹¹ m			

表8. 国際単位系に属さないが国際単位系と

	伊用されるその他の単位					
名称			記号	SI 単位であらわされる数値		
海		里		1 海里=1852m		
1	ツ	ŀ		1 ノット=1海里毎時=(1852/3600)m/s		
ア	-	IV	а	1 a=1 dam ² =10 ² m ²		
ヘク	タ・	- N	ha	$1 \text{ ha}=1 \text{ hm}^2=10^4 \text{m}^2$		
バ	-	IV	bar	1 bar=0.1MPa=100kPa=1000hPa=10 ⁵ Pa		
オングストローム Å			Å	1 Å=0. 1nm=10 ⁻¹⁰ m		
バ	_	ン	b	$1 \text{ b}=100 \text{ fm}^2=10^{-28} \text{m}^2$		

表9 固有の名称を含むCGS組立単位

衣9. 固有の名称を含むGGA組立単位								
名称	記号	SI 単位であらわされる数値						
エル	グ erg	1 erg=10 ⁻⁷ J						
ダイ	ン dyn	$1 \text{dyn} = 10^{-5} \text{N}$						
ポーア	ズ P	1 P=1 dyn • s/cm ² =0.1Pa • s						
ストーク	ス St	1 St $=1 \text{ cm}^2/\text{s}=10^{-4}\text{m}^2/\text{s}$						
ガウ	ス G	1 G ≙10 ⁻⁴ T						
エルステッ	ド 0e	1 Oe ≙(1000/4π)A/m						
マクスウェ	ルレ Mx	1 Mx ≙10 ⁻⁸ Wb						
スチル	ブsb	$1 \text{ sb } = 1 \text{ cd/cm}^2 = 10^4 \text{ cd/m}^2$						
ホ	Ի ph	1 ph=10 ⁴ 1x						
ガ	ル Gal	$1 \text{ Gal} = 1 \text{ cm/s}^2 = 10^{-2} \text{ m/s}^2$						

表10. 国際単位に属さないその他の単位の例							
名称					記号	SI 単位であらわされる数値	
キ	ユ		IJ	ĺ	Ci	1 Ci=3.7×10 ¹⁰ Bq	
\mathcal{V}	ン	ŀ	ゲ	\sim	R	$1 R = 2.58 \times 10^{-4} C/kg$	
ラ				F	rad	1 rad=1cGy=10 ⁻² Gy	
\mathcal{V}				A	rem	1 rem=1 cSv=10 ⁻² Sv	
Х	線		単	位.		1X unit=1.002×10 ⁻⁴ nm	
ガ		$\boldsymbol{\mathcal{V}}$		7	γ	$1 \gamma = 1 nT = 10^{-9}T$	
ジ	ヤン	/ 7	ス キ		Jу	$1 \text{ Jy}=10^{-26} \text{W} \cdot \text{m}^{-2} \cdot \text{Hz}^{-1}$	
フ	エ		ル	Ξ		1 fermi=1 fm=10 ⁻¹⁵ m	
メートル系カラット				ット		1 metric carat = 200 mg = 2×10^{-4} kg	
ŀ				ル	Torr	1 Torr = (101 325/760) Pa	
標	準	大	気	圧	atm	1 atm = 101 325 Pa	
力			IJ	-	cal		
Ξ	ク		П	\sim	μ	$1 u = 1 u = 10^{-6} m$	

この印刷物は再生紙を使用しています