Sample user code

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Sample user codes (Prepared with Text)

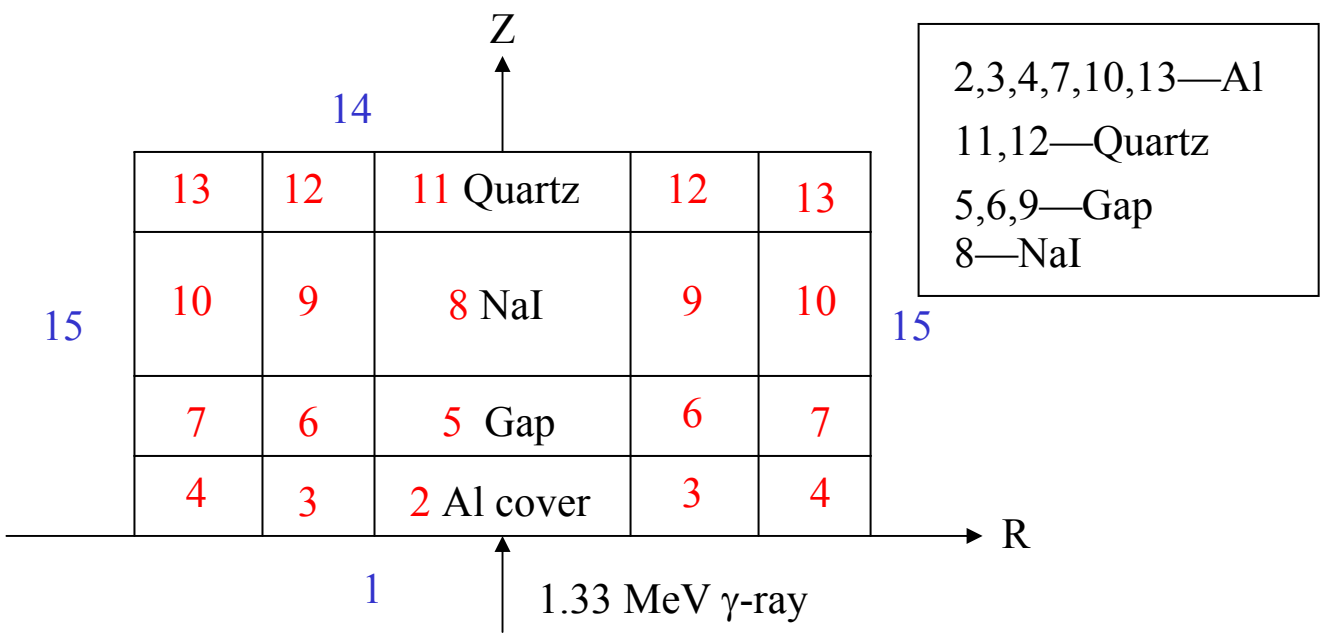
Name of user code	Geometry	Quantity calculated	Trajectories display system used
ucrz_nai.f	Cylinder-plane	NaI detector response	Not used
uccg_nai.f	CG	Same above	Not used
ucxyz_phantom.f	Voxel	Dose distribution inside phantom	PICT32
uccg_phantom.f	CG	Same above	CGview

Other sample user code prepared

- Define material used, assign material to each region, geometry, source particle conditions (energy, direction, type of particle etc.) etc. at the main program.
  - ucshield.f – corresponding to ucshield.mor
  - ucphantom_rec.f – corresponding to ucphantom_rec.mor
- Cylinder-slab geometry
  - ucrz_sampl4.f – cylinder-slab version ucsampl4.mor
- Voxel geometry
  - ucxyz_dose.f – corresponding to xyzdose.mor

ucrz_nai.f

- Response calculation of NaI detector with cylinder-plane geometry



Include lines and specification statements

- The size of arguments is defined at other files and included by using 'include line'.
- Various commons used inside egs5 are also included by the same way.
  - Include files related directory with egs5 are put on the sub-directory ('include' directory) of egs5 directory.
  - Those for
  - each user including geometry related are put on the subdirectory ('user_auxcommon' directory) of user directory.

```
include 'include/egs5_h.f'              ! Main EGS "header" file

 include 'include/egs5_edge.f'
 include 'include/egs5_media.f'
 include 'include/egs5_misc.f'
 include 'include/egs5_switches.f'
 include 'include/egs5_uphiot.f'
 include 'include/egs5_useful.f'
 include 'include/randomm.f'
```

egs5 commons.

Include here when variables including in these commons are used at the program unit like main program.

```
include 'user_auxcommons/aux_h.f'   ! Auxiliary-code "header" file

 include 'user_auxcommons/cyldta.f'
 include 'user_auxcommons/edata.f'
 include 'user_auxcommons/etaly1.f'
 include 'user_auxcommons/georz.f'
 include 'user_auxcommons/instuf.f'
 include 'user_auxcommons/lines.f'
 include 'user_auxcommons/pladta.f'
 include 'user_auxcommons/watch.f'
```

Non egs5 commons like geometry related.

In include/egs5_h.f

```
! Maximum number of regions allocated
      integer MXREG
parameter (MXREG = 10649)
```

Change this value if you want use more region.

include/egs5_misc.f

```
 common/MISC/                          ! Miscellaneous COMMON
     * rhor(MXREG), dunit,
     * med(MXREG),iraylr(MXREG),lpolar(MXREG),incohr(MXREG),
     * iprofr(MXREG),impacr(MXREG),
     * kmpi,kmpo,noscat

      real*8
     * rhor,dunit

      integer
     * med,iraylr,lpolar,incohr,iprofr,impacr,kmpi,kmpo,noscat
```

```
 common/totals/                          ! Variables to score
* depe,deltae,spg(1,50),spe(1,50),spp(1,50),nreg
 real*8 depe,deltae,spg,spe,spp
 integer nreg

   real*8                                 ! Local variables
* availke,avpe,avph,avspe,avspg,avspp,avte,ekin,etot,
* desci2,pef,rnnow,sigpe,sigph,sigspe,sigspg,sigspp,
* sigte,tef,totke,wtin,wtsum

 real*8
* ph(50),phpb(50,50),spgpb(1,50,50),spepb(1,50,50),
* spppb(1,50,50),pefpb(50),tefpb(50)

 real                                   ! Local variables
* elow,eup,rdet,rtcov,rtgap,tcov,tdet,tgap

 real
* tarray(2),tt,tt0,tt1,cputime

 integer
* i,icases,idin,ie,imed,ireg,isam,isot,
* j,k,n,nbatch,ncaspb,nd,ndet,nlist,nofbat
```

Open statements

- Due to the new feature that pegs is called inside each user code, it must be careful to the unit number used.
- The unit number from 7 to 26 are used inside 'pegs' and close at the end of 'pegs'. These units, therefore, must be re-open after calling pegs.
- It is better not to use these unit in the user code.
- Unit number of write statements related to plotxyz.f which used to output trajectory information, changed from 9 to 39.

Call subroutine getrz

- getrz (name of subroutine and its function is different depending on each user code) is the new subroutine used to run pegs as a part of user code and call subroutine hatch.
- In the subroutine getrz, material used, egs5 cut-off energy, various option flag, geometry related data etc. will be set by reading data from unit 4.
- If uin=vin=win=0.0, is set isot to 1 as the flag for isotropic source at the main program.

Call shower

- Number of histories per batch (ncaspb) is calculated from batch number (nbatch and number of histories (ncases).
- Subroutine shower is called ncasepb times at each batch and repeated tt nbatch times.
- Source energy is sampled based on the data read from unit 4 at subroutine getrz.
- If some energy deposited at NaI, adds weight as total efficiency. If its
- energy is larger than 99.9% of source kinetic energy, treat as total absorption peak and adds weight as peak efficiency.
- Bin number corresponding absorbed energy is calculated to assign pulse height.

Source energy sampling

- isamp=0
  - Use ekin as an monoenergey source.
- isamp=1
  - Sampl from discrete type distribution (Ex. Gamma-ray from a radioisotope)
- isamp=2
  - Sampl using cdf calculated at getrz from pdf data as continuous distribution.
- isamp=3
  - Sample energy as uniformly distribution from energy region considered and apply pdf corresponding sampled energy as a weight.

Estimate statistical uncertainty

- There are 2 ways to estimate uncertainty of obtained, x. One is the way used at MCNP and other at MORCE-CG.
- The way used at MCNP
  - Assume that the calculation calls for *N* incident particle histories.
  - Assume that *x_i* is the result at the *i*-th history.

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$ Average value of x_i

$$s^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - x)^2 \approx \overline{x^2} - (\bar{x})^2 ; (\overline{x^2} = \frac{1}{N}\sum_{i=1}^{N} x_i^2)$$ Variance associated with distribution of x_i

$$s_{\bar{x}}^2 = \frac{1}{N}s^2 \approx \frac{1}{N}[\overline{x^2} - \bar{x}^2]$$ Variance associated with distribution of $\bar{x}$

$$R = \frac{s_{\bar{x}}}{\bar{x}} \approx [\frac{1}{N}(\frac{\overline{x^2}}{\bar{x}^2} - 1)]^{1/2}$$ Statistical error

The way used at MORSE-CG

- Assume that the calculation calls for *N* incident particle histories.
- Split the N histories into *n* statistical batches of N/n histories each.
- The calculated quantity for each of these batches is called $*x*_*i*$.

$$\bar{x} = \frac{1}{n}\sum_{j=1}^{n} x_j$$ Mean value of x_j

$$s_x^2 = \frac{1}{n-1}\sum_{j=1}^{n}(x_j - x)^2 = \frac{1}{n-1}\sum_{j=1}^{n}(x_j^2 - \bar{x}^2)$$ Variance associated with distribution of x_j

$$s_{\bar{x}}^2 = \frac{s_x^2}{n}$$ Standard variance of the mean

$$FSD = \frac{s_{\bar{x}}}{\bar{x}}$$ Fractional standard deviation

The uncertainty estimation used at ucrz_nai.f

- Calculate FSD using the way used at MORCE-CG.
- Average value $\bar{x}_i$ Is calculated at the end of each batch.

```
!  Calculate average value for this BATCH
     do ie=1,50
       phpb(ie,nofbat) = ph(ie) /ncaspb
       ph(ie)=0.D0
     end do
     pefpb(nofbat)=pef / ncaspb
     tefpb(nofbat)=tef /ncaspb
     pef=0.D0
     tef=0.D0
     do nd=1,ndet
       do ie=1,50
         spgpb(nd,ie,nofbat)=spg(nd,ie)/ncaspb !photon spectrum
         spepb(nd,ie,nofbat)=spe(nd,ie)/ncaspb !electron spectrum
         spppb(nd,ie,nofbat)=spp(nd,ie)/ncaspb !positron spectrum
         spg(nd,ie)=0.D0
         spe(nd,ie)=0.D0
         spp(nd,ie)=0.D0
       end do
     end do
```

Puse-height distribution

Peak efficiency

Total efficiency

Spectrum entering to NaI from ouside the detector

Analyze the obtained results

- Average values and their statistical uncertainty FSD are calculated form the average results per batch.

```
!     ---------------
!     Peak efficiency
!     ---------------
      avpe = 0.D0
      desci2 = 0.D0
      do j = 1, nbatch
        avpe = avpe + pefpb(j)/nbatch
        desci2 = desci2 + pefpb(j)*pefpb(j)/nbatch
      end do
      sigpe = sqrt((desci2 - avpe*avpe)/(nbatch-1))
      avpe = avpe*100.0
      sigpe = sigpe*100.0
      write(6,210) avpe,sigpe
210   FORMAT(' Peak efficiency =',G15.5,'+-',G15.5,' %')
```

Subroutine getrz

- Subroutine getrz used to define material used, its density, egs5 cut-off energy, various optional flag applied to each region, data for cylinder-plane geometry related etc. and call subroutine hatch.

```
! -----------------
! Record 1: title
! -----------------
      read(4,101) title
 101  FORMAT(80A1)
      write(6,102) title
 102  FORMAT(' TITLE:'/1X,80A1/)

! ------------------
! Record 2: nmed
! ------------------
      read(4,*) nmed
      if (nmed .gt. MXMED) then
        write(6,104) nmed
 104    FORMAT(' *** Stopped in GetRZ with nmed=',I5,' > MXMED')
        stop
      end if
      write(6,105) nmed
 105  FORMAT(' nmed=',I5,/)
```

Title (within 80 characters)

Number of materials used.

Check not to exceed the maximum value assigned.

```
! ------------------
! Record 3: media
! ------------------
     do i=1,nmed
       read(4,106) (media(j,i),j=1,24)
 106    FORMAT(24A1)
       write(6,107) i,(media(j,i),j=1,24)
 107    FORMAT(' MEDIUM=',I5,' ==> ',24A1)
     end do
```

Read material name at each line with 24 characters.

The name must be included material created at pegs.

```
! --------------------
! Record 4: ncyl, nplan
! --------------------
     read(4,*) ncyl, nplan

     if (ncyl .gt. MXCYLS) then
       write(6,114) ncyl
 114    FORMAT(' *** Stopped in getrz with ncyl=',I5,' > MXCYLS')
       stop
     end if
```

Number of cylinders (ncyl)

Number of planes (nplan)

Check number of planes not to exceed value set by parameter satement

Check plane number by the same way.

```
!     ------------------------
      nreg = (nplan-1)*ncyl+3
      irz = nreg - 3
!     ------------------------

      if (nreg .gt. MXREG) then
        write(6,118) nreg
 118    FORMAT(' *** Stopped in getrz with nreg=',I5,' > MXREG')
        stop
      end if
      write(6,119) nreg
 119  FORMAT(/,' number of region (nreg) =',I5,/,
     *        ' nreg includs front, back and outside cylinder')
```

Calculate region number necessary (nreg) from the number of cylnders and planes.

Before the first plane, after the last plane and outside the largest cylinder are treated as the different region.

Check nreg not exceed the maximum region set by parameter statement.

```
! --------------
! Record 5: cyrad
! --------------
      write(6,120)
 120  FORMAT(/,' Input radius of cylinder:',/)

      do i=1,ncyl
        read(4,*) cyrad(i)
        cyrad2(i) = cyrad(i)**2
        write(6,122) i,cyrad(i)
 122      FORMAT(5X,'i=',I3,5X,'cyrad=',G15.7,' cm')
      end do

! -------------
! Record 6: tpl
! -------------
      write(6,127)
 127  FORMAT(/,' Input boundaries in the Z direction:',/)

      do k=1,nplan
        read(4,*) zpl(k)
        write(6,129) k,zpl(k)
 129    FORMAT(5X,'k=',I3,5X,'zpl=',G15.7,' cm')
      end do
```

Read r a radius of cylinder from inner side.

Calculate radius square which is use at howfar.

Read the intersection point of Z-axis and each plane which is perpendicular with Z-axis.

```
 read(4,142) medtmp,rhotmp,ecutin,pcutin
142      FORMAT(I10,3F10.3)
         if (medtmp.ne.0) then
! ---------------------------------------
! Record 7a: ipeangsw,iedgesw,iraysw,ipolarsw,
!            incohrsw,iprofrsw,impacrsw
! ---------------------------------------
           read(4,145) ipeangsw,iedgesw,iraysw,ipolarsw,incohrsw,
     *     iprofrsw,impacrsw
145        FORMAT(7I5)
```

At first, set the same material for all regions at each Z-bin.

Read material number, its density and cut-off energy.

If density or cut-off energy is 0.0, default value is used.

If material is not vacuum (0), read various option data.

Various options can be applied to each region

iphter(irl)	Switches for PE-angle sampling
iedgfl(irl)	K & L-edge fluorescence
iraylr(irl)	Rayleigh scattering
lpolar(irl)	Linearly-polarized photon scattering
incohr(irl)	S/Z rejection
iprofr(irl)	Doppler broadening
impacr(irl)	Electron impact ionization

```
! ------------------------------------------------------------
!  Record 8  nzbin, nrbin, meptmp, rhotmp, ecutin, pcutin
!------------------------------------------------------------
!     ------------------------------------------
!     Check exception. nzbin=0 means end.
!     ------------------------------------------
160    continue
      read(4,162) nzbin,nrbin,medtmp,rhotmp,ecutin,pcutin
162    FORMAT(3I5,3F10.3)
      if(nzbin .eq. 0) go to 170
!     ----------------
!     Set exception.
!     ----------------
      irl=(nzbin-1)*ncyl+nrbin+1
      med(irl)=medtmp
```

Read material number etc. for the region having different ones from preset values at each Z-bin.

Region number is assigned by Z-bin and R-bin.

If Z-bin equal 0, it mean s the end of assign.

If material assigned is not vacuum, read various option data.

```
! --------------------
! Record 9: xin,yin,zin
! --------------------
      read(4,*) xin,yin,zin

! --------------
! Record 10: irin
! --------------
      read(4,*) irin

! ---------------------
! Record 11: uin,vin,win
! ---------------------
      read(4,*) uin,vin,win
```

Source position

Region number of source osition

Directional cosine of source particle

If uin=vin=win=0.0, treat as isotropic source.

Read 2 random number seeds for RANECU

```
! -----------------
! Record 12: ixx,jxx
! -----------------
      read(4,*) ixx,jxx
      if (ixx .eq. 0)  ixx = 123457            ! Default seed
      if (jxx .eq. 0)  jxx = 654321            ! Default seed
      write(6,210) ixx,jxx
210   FORMAT(/,' ixx=',I12,5X,'jxx=',I12,
     *       ' (starting random-number seeds)')

!     ---------------------------------
!     Save the starting random-number seeds
!     ---------------------------------
      iseed1=ixx
      iseed2=jxx
```

If last seeds is set as starting seeds, it is possible to connects to the previous run,

If it is possible to find stating seeds of history to cause some error, it will be useful to set these seeds as ixx and jxx for finding the reason of errors.

```
! ----------------
! Record 13: ncases
! ----------------
      read(4,*) ncases
      write(6,220) ncases
220   FORMAT(/,' ncases=',I12)

! --------------------------
! Record 14: ekein,iqin,isamp
! --------------------------
      read(4,*) ekein,iqin,isamp
```

History number

Maximum kinetic energy of source particle

Charge of source particle

Type of source

Isamp=0 : monoenegy source (ekein)

=1 : Sample from discrete type source（Ex. γ-rays from radioisotope）.

=2 : Sample from continuous type source using cdf calculated by pdf read.

=3 : Energy sampled uniformly between considered energy region.

Pdf is used as the weight.

```
! ---------------------
! Record 15: iwatch
! ---------------------
      read(4,*) iwatch

! -----------------------------------
! Record 16: ibrdst,iprdst,ibrspl,nbrspl
! -----------------------------------
      read(4,*) ibrdst,iprdst,ibrspl,nbrspl

      if (ibrspl .gt. 0) then
        if (nbrspl .gt. 0) then
          fbrspl = 1.0/float(nbrspl)
        else
          write(6,420) ibrspl,nbrspl
420       FORMAT(//,' Stopped in GetRZ with IBRSPL=',I5,' and NBRSPL=',
     *    I5)
          stop
        end if
      end if
```

Read iwatch option flag

0=off, 1=each interaction, 2=each step

Switches for bremsstrahlung production ANGLE SAMPLING,
brdst=0 No (use default: theta=m/E)
1 Yes (recommended)

Switches for pair production ANGLE SAMPLING
iprdst=0 No (use default: theta=m/E)
1 Yes (low-order distribution)
2 Yes (recommended)

Splitting option flag

ibrspl not 0 : split to nbrspl aprticles

```
! ------------------------------
! Record 17: estepe,estepe2
! ------------------------------
      read(4,*) estepe, estepe2
```

Parameters used at charged particle transport

This will be explained in detail by Alex F. Bielajew and Scot J. Wildernam.

Function of ausgab

- Function of ausgab is to score information that user want to calculate.
- In this user code, energy deposition inside NaI detector and each particle spectrum entering from outside the detector are scored.

```
!     ------------------------------------------
!     Score energy deposition inside NaI detector
!     ------------------------------------------
      if (med(irl). eq. 1) then
        depe = depe + edepwt
```

If the medium number at this region (med(irl)) is 1, it means particle is inside NaI detector.

Function of ausgab

```
!     ------------------------------------------------------------
!     Score particle information if it enters from outside
!     ------------------------------------------------------------
      if (irl .ne. irold .and. iarg .eq. 0) then
        if (iql .eq. 0) then              ! photon
          ie = e(np)/deltae +1
          if(ie .gt. 50) ie = 50
          spg(1,ie) = spg(1,ie) + wt(np)
        elseif (iql .eq. -1) then         ! electron
          ie = (e(np) - RM)/deltae +1
          if(ie .gt. 50) ie = 50
          spe(1,ie) = spe(1,ie) + wt(np)
        else                              ! positron
          ie = (e(np) - RM)/deltae +1
          if(ie .gt. 50) ie = 50
          spp(1,ie) = spp(1,ie) + wt(np)
        end if
      end if
    end if
```

If the region number changes due to transport of particle, it means that this particle enters from outside.

Function of howfar

- Howfar is the subroutine to transfer information related to geometry.
- At subroutine howfar, a distance to the boundary of region is checked.
- If the distance to the boundary is shorter than the distance to the next point,
  - the distance to the next point is replaced with the distance to the boundary,
  - new region, irnew, is set to the region number to which particle will enter.
- If idisc is set to 1 by user, the treatment to stop following will be done in this subroutine.
- Various geometry related subroutines are prepared for egs5.
- It will be explained in detail at the lecture of “How to write geometry”.