

Los Alamos

NATIONAL LABORATORY

memorandum

Applied Physics Division

X-5: Diagnostics Applications

To/MS: Distribution
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Symbol: X-5:RN(U)-JSH-01-17
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Subject: MCNP4C3 - 3/22/01

MCNP4C3^{TM1 2} - 03/22/01 is a correction patch to MCNP4C2³. The MCNP4C3 correction will be posted to the WWW and will be updated periodically as MCNP4C3 - xx/xx/xx with different load dates as required if further bugs are found.

The MCNP4C3 correction patch is attached. The corrections are ranked according to the seriousness of the problem. None of the bugs found is serious enough to provide incorrect answers except in PVM mode.

Serious problems:

1. Geometry plots fail when not using XLIB graphics. *Affects geometry plotting on some PCs.* (GWM) 03/01/01
2. Cannot plot electron cross section data (error introduced when photoneutrons were added to MCNP4C2). (RCL/JSH) 02/28/01
3. Macrobody surfaces with facet numbers greater than .5 could not be specified on the SDEF card. (JSH) 03/13/01 \$20 awarded Sander Nievaart, Technical University, Delft, Netherlands X-5:JSH-01-28(U)
4. An array could overflow when using macrobodies and writing on MCTAL files causing a crash or bad output. (GWM/JSH) 02/28/01
5. The computer time used is incorrectly reported in the problem summary table in all previous MCNP versions. *For sequential problems the only effect is that the summary table time is reported about twice as large as the correct time at the problem end. For PVM the figure-of-merit and statistical checks are also affected.* (GWM) 03/21/01
6. Prevent a negative square root in rare cases with superimposed mesh weight windows. (TEB/JAF) 02/07/01
7. DEC compiler error workaround when reading some superimposed mesh weight windows. (JSH) 02/15/01

¹MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory

²J. F. Briesmeister, Ed., "MCNP - A General Monte Carlo N-Particle Transport Code, Version 4C," LA-13709-M, Los Alamos National Laboratory (April 2000)

³J. S. Hendricks, "MCNP4C2," X-5:RN(U)-JSH-01-01, LA-UR-01-858 (30 January, 2001)

PVM Bugs:

1. Fix a bug on the tasks execution line, so that the proper warnings messages are issued if the code is incorrectly compiled or initialized for various modes of multiprocessing or multitasking or both. *Affects warning messages. Also, the attached correction patch now allows "tasks N" instead of requiring "tasks NxM" or "tasks MxN" for PVM or threads alone.* (GWM) 03/07/01
2. PVM bug with acode. *Causes crash.* (GWM) 03/11/01
3. Fix a PVM bug when counting detector/DXTRAN large scores. *Affects DD card Russian roulette game and diagnostic prints.* (GWM) 03/09/01
4. Prevent backing up expired histories when multiprocessing but not in history-running part of code (MCRUN). *That is, an EXPIRE error during initiation will now correctly cause MCNP to stop.* (GWM) 03/08/01
5. PVM bug with source weight. *Affects printout only.* (GWM) 03/13/01
6. Collect other-side cell data for output/continue-runs. *Affects problem efficiency.* (GWM) 03/12/01
7. Remove spurious PVM warning messages. *Harmless.* (GWM) 03/12/01
8. Write multiprocessing master messages based on MCT parameter on PRDMP card. *Causes spurious messages when comparing OUTF files.* (GWM) 03/10/01

Minor bugs:

1. Correct setting of dbcn(8). *MCNP4C2 error only, causing histories to start with random number of wrong history. Affects dbcn(8) option only.* X-5:REP-00-117 (REP/JSH) 09/14/00
2. Do not use weight windows values from the superimposed importance mesh if outside the mesh. *Makes variance reduction inefficient if the superimposed mesh does not overlap the entire problem geometry.* (TEB/JAF) 02/08/01
3. Correct warning message when generating or using multigroup importances in the multigroup mode. (JSH) 02/15/01
4. Print macrobody surfaces in first 50 histories. *Harmless.* (JSH) 03/13/01
5. Remove kcode settle time, cpk, from tally signal/noise ratio. *Harmless — affects only signal/noise printout.* (JSH) 03/21/01
6. Correct print table 190 print. *Harmless — affects only printout of superimposed mesh weight window reference cell weight.* (JSH) 01/31/01
7. Clean up cross section plotting false warning. *Harmless.* (JSH) 03/01/01
8. Corrections to the undocumented recursive Monte Carlo feature which is in MCNP4C2 under development.

MCNP4C3 - 03/22/01 Correction Patch

```
*/ Create MCNP4C3 from MCNP4C2                                03/22/01
*/ XBUG denotes serious bug.
*/ dbcn(29).eq.0.to track 4c2 (inverse dbcn(20))
*ident zc4c3 ----- comdeck zc
*d,zc4c2.1                                                    <21>
    parameter (kod='mcnp',ver='4c3',loddatt='03/22/01')
*ident cm4c3 ----- comdeck cm
*/ Fix cpu timing bugs. Eliminate cp0,cpa                    (GWM/JSH) 03/22/01
*d,cm4c.27                                                    <119>
    parameter (nephcm = 12*(1)+1*(4)+1*(11)+1*(mcpu)
*d,cm.21                                                      <125>
    equivalence (cp1,gephcm),(ichan,jepgcm)
*d,cm4c.107                                                  <211>
    common /epgcm/ cp1,cp2(mcpu),cp3,ctme,fpf,freq,
*ident mc4c3 ----- mcnp
*/ Fix cpu timing bugs. Eliminate cp0,cpa                    (GWM/JSH) 03/22/01
*i,mc.42 after start up                                       <709>
c
c    initialize cpu clock.
    call secnd(tq)
*d,mc.143 call secnd(cpa)                                       <804>
*/ Fix cpu timing bugs.                                       (GWM) 03/22/01
*d,mc4c.34,mc4c.35                                           <897>-<898>
*d,mc4c.36                                                    <900>
    1 (tq+cp3)/60.
*ident em4c3 ----- exemes
*/ Fix a bug on the tasks execution line.                    (GWM) 03/07/01
*d,em4c.14,em4c.15                                           <1136>-<1137>
*d,em4c.17,em4c.29                                           <1139>-<1154>
*if -def,multt.and.multp
c
c    no multiprocessing.
    if(ntasks.gt.1.or.ltasks.gt.1)call expire(0,'exemes',
    1 'multiprocessing is unavailable in this compilation.')
*endif
*if def,multt
*if -def,multp,4
c
c    multitasking only.
    if(j.gt.0.and.ltasks.gt.1)call expire(0,'exemes',
    1 'message-passing is unavailable in this compilation.')
*endif
*if def,multp
```

```
*if -def,multt,8
c
c      message-passing only.
      if(j.eq.0)then
          ltasks=ntasks
          ntasks=1
      endif
      if(j.gt.0.and.ntasks.gt.1)call expire(0,'exemes',
1 'multitasking is unavailable in this compilation.')
```

```
c
c      message-passing with or without multitasking.
      if(ltasks.gt.1)then
          if(mynum.lt.0)call expire(0,'exemes',
1 'pvm not initialized, invoke pvm daemon first.')
```

```
          call mnum(n,k)
          if(k.eq.0.and.n.lt.ltasks)call erprnt(1,2,2,n,ltasks,0,0,-1,
1 '5honly ,i3,31h host(s) available through pvm,,i3, '//
2 '17h tasks requested.')
```

```
          lchnk=min(10000000,(625/ltasks)*100000)
      endif
*endif
*if def,multt.and.multip
c
c      multitasking and message-passing.
      if(j.eq.0)call expire(0,'exemes',
1 'format of tasks keyword is #x# - see manual.')
```

```
*endif
*ident qj4c3 ----- qttyin
*/ Fix cpu timing bugs. Eliminate cp0,cpa          (GWM/JSH) 03/22/01
*d,qj4a.32,qj4a.34          <1248>-<1250>
      if(ia.lt.0)write(jtty,ha)(t)/60.,nps,nch(1)+nch(2)+nch(3)
      if(ia.eq.0)write(jtty,ha)(t)/60.
      if(ia.gt.0)write(jtty,ha)(t)/60.,ia
*ident ex4c3 ----- expire
*/ Prevent backing up expired histories when multiprocessing but not
*/ in history-running part of code (mcrun)          (GWM) 03/08/01
*d,ex4c.1          <1721>
      if(iovr.eq.4.and.(ntasks.gt.1.or.ltasks.gt.1))return
*ident zw4c3 ----- wwfile
*/ DEC compiler error workaround.          (JSH) 02/15/01
*d,zw4c.13          <2428>
      kh=kdarg(ha,jc,0,hb,r)
      if(kh.gt.0.and.jk.ne.0)go to 20
*ident vi4c3 ----- avrwi
*/ Do not use WWG mesh WW values if outside mesh.    (TEB/JAF) 02/08/01
```

```
*d,vi4c.249 <2827>
    call avrxyz(dc,mi,-one,ie)
*d,vi4c.264 <2842>
    call avrxyz(cc,mi,-one,ie)
*ident rmi4c3 ----- rmcini
*/ correct loop over ip (TEB) 01/30/01
*i,rmi.6 <2872>
    do 193 ip=1,mipt
    nw=nwwm*mww(ip)
*i,rmi.29 <2895>
    193 continue
*ident ce4c3 ----- chekit
*/ Spurious fatal error for some SDEF macrobody surfaces. (JSH) 03/13/01
*/ $20 awarded Sander Nievaart, Tudelft, Netherlands X-5:JSH-01-28(U)
*d,ce.232 <5194>
    i=namchg(m2c,abs(iitm))
    if(m2c.eq.2.and.kitm.eq.1)i=namchg(m2c,int(abs(ritm)))
    if(i.le.0)call erprnt(2,1,1,abs(iitm),0,0,0,0,
*ident pl4c3 ----- plotg
*/ Non-xlib geometry plots fail. XBUG (GWM) 03/01/01
*d,pl4c2.2 <16985>
    nq=0
*ident mg4c3 ----- mgimps
*/ Correct typo. (JSH) 02/15/01
*d,mg4b.9 <22006>
    1 '53hweight-windows from wwinp, other-way fluxes disabled.')
```

```
*ident mr4c3 ----- mcrun
*/ Fix cpu timing bugs. (GWM) 03/22/01
*d,mr4c.5,mr4c.6 <24193>-<24194>
    call secnd(t1)
*/ Fix cpu timing bugs. Eliminate cp0,cpa (GWM/JSH) 03/22/01
*d,mr4b.2 <24205>
    10 write(jtty,20)lf11,lf11*8/ndp2,t1/60.
*d,mr4b.6 <24209>
    1 t1/60.,aid
*ident tn4c3 ----- trnspt
*/ Fix cpu timing bugs. (GWM) 03/22/01
*i,tn.13 <24291>
    call secnd(t1)
    cp2(ktask+1)=t1
*d,tn4c.3 <24312>
    if(mynum.gt.0.and.kbp.lt.0)go to 30
*i,tn4a.11 <24355>
*if def,multp,1
    if(mynum.gt.0.and.kbp.lt.0)go to 75
```

```
*i,tn.117 <24391>
  call secnd(t2)
  cp1=cp1+(t2-cp2(ktask+1))/ntasks
  cts=cts+t2-cp2(ktask+1)
*i,tn.118 <24392>
  call secnd(t2)
  if(ktask.eq.0)cp3=cp3-(t2-t1)
  cp3=cp3+t2-cp2(ktask+1)
*ident ut4c3 ----- utask
*/ Fix PVM bug when counting detector/DXTRAN large scores.(GWM) 03/09/01
*i,ut4a.15 <24495>
c
c      backup l-pointer values for use in msgtsk.
      do 56 j=1,ndnd
56      ddn(kddn+22,j)=ddn(lddn+22,j)
      do 57 k=1,mxdx*min(1,nxn)
      do 57 j=1,mipt
57      dxd(kxd+j,22,k)=dxd(ldxd+j,22,k)
*ident me4c3 ----- msgcon
*/ Write multiprocessing master messages based on MCT. (GWM) 03/10/01
*/ Should use -2 in INP?? files and then change these to if(mct.ge.-1).
*d,me4c.26,me4c.27 <24767-24768>
      if(mct.ge.0)write(iuo,'(/16h master starting,i8,3h by,i8,
      1 10h subtasks ,a19)')ltasks,ntasks,hd
*d,me4c.78,me4c.79 <24819-24820>
*d,me4c.106 <24847>
*d,me4c.175 <24916>
      if(mct.ge.0)write(iuo,'(27hmaster set rendezvous nps =,i10,5x,
      1 a19)')nps+n,hd
*/ PVM bug with acode. (GWM) 03/11/01
*d,me4c.194 <24935>
      if(nsr.eq.71.and.nss.eq.0)call mputd(fso(lfso+1),6*msrk,i)
*/ Fix cpu timing bugs. (GWM) 03/22/01
*d,me4c.276 <25016>
*/ Remove spurious PVM warning messages. (GWM) 03/12/01
*d,me4c.280,me4c.285 <25020-25025>
c
c      save all variables used to count warning messages.
      n0=nerr
      n1=netb(1)
      n2=netb(2)
      n3=nwse
      n4=nwst
      n5=nwsg(1)
      n6=nwsg(2)
```

```

n7=nwsg(3)
n8=nwsb
n9=jrad
m1=nesm
m2=nsom
m3=nppm
m4=npnm
m5=nkrp
m6=jtlx
*d,me4c.336,me4c.349 <25076-25089>
  call mgeti(n,1,i)
  nerr=nerr+n-n0
  call mgeti(n,1,i)
  netb(1)=netb(1)+n-n1
  call mgeti(n,1,i)
  netb(2)=netb(2)+n-n2
  call mgeti(n,1,i)
  nwse=nwse+n-n3
  call mgeti(n,1,i)
  nwst=nwst+n-n4
  call mgeti(n,1,i)
  nwsg(1)=nwsg(1)+n-n5
  call mgeti(n,1,i)
  nwsg(2)=nwsg(2)+n-n6
  call mgeti(n,1,i)
  nwsg(3)=nwsg(3)+n-n7
  call mgeti(n,1,i)
  nwsb=nwsb+n-n8
  call mgeti(n,1,i)
  jrad=jrad+n-n9
  call mgeti(n,1,i)
  nesm=nesm+n-m1
  call mgeti(n,1,i)
  nsom=nsom+n-m2
  call mgeti(n,1,i)
  nppm=nppm+n-m3
  call mgeti(n,1,i)
  npnm=npnm+n-m4
  call mgeti(n,1,i)
  nkrp=nkrp+n-m5
  call mgeti(n,1,i)
  jtlx=jtlx+n-m6
*d,me4c.364,me4c.373 <25104-25113>
*/ Fix PVM bug when counting detector/DXTRAN large scores.(GWM) 03/09/01
*d,me4c.380 <25120>
```

```
330 ddn(lddn+22,j)=ddn(lddn+22,j)+dble(nint(a))
*d,me4c.384 <25124>
340 dxd(ldxd+j,22,k)=dxd(ldxd+j,22,k)+dble(nint(a))
*/ Collect other-side cell data for output/continue-runs. (GWM) 03/12/01
*i,me4c.393 <25133>
    call mgeti(laj(1laj+1),(mlaj+mx)*mtasks,i)
    call mgeti(lcaj(1lcj+1),(mlja+1)*mtasks,i)
*/ Fix cpu timing bugs. (GWM) 03/22/01
*i,me4c.403 <25143>
    call mgeti(ntc,1,i)
    call mgeti(ntc1,1,i)
*i,me4c.461 <25201>
    cs=cts
*d,me4c.468 <25208>
    call mgetd(a,1,i)
    cts=cts+a-cs
*/ Fix PVM bug when counting detector/DXTRAN large scores.(GWM) 03/09/01
*d,me4c.483,me4c.491 <25223-25231>
470 continue
*ident mh4c3 ----- msgtsk
*/ Fix cpu timing bugs. (GWM) 03/22/01
*i,mh4c.17 <25275>
    call secnd(t1)
*d,mh4c.24 <25282>
*/ PVM bug with acode. (GWM) 03/11/01
*d,mh4c.141 <25399>
    if(nsr.eq.71.and.nss.eq.0)call mgetd(fso(lfso+1),6*msrk,i)
*/ Remove spurious PVM warning messages. (GWM) 03/12/01
*d,mh4c.150,mh4c.151 <25408-25409>
*d,mh4c.161,mh4c.165 <25419-25423>
*/ PVM bug with source weight. (GWM) 03/13/01
*d,mh4c.182,mh4c.185 <25440-25443>
170 do 180 i=1,nvarsw
180 gvarcm(i)=0.
    wgts(1)=huge
*/ Remove spurious PVM warning messages. (GWM) 03/12/01
*d,mh4c.319,mh4c.324 <25577-25582>
    call mputi(nerr,1,i)
    call mputi(netb,2,i)
    call mputi(nwse,1,i)
    call mputi(nwst,1,i)
    call mputi(nwsg,3,i)
    call mputi(nwsb,1,i)
    call mputi(jrad,1,i)
    call mputi(nesm,1,i)
```



```
      call mputi(nsom,1,i)
      call mputi(nppm,1,i)
      call mputi(npnm,1,i)
      call mputi(nkrp,1,i)
      call mputi(jtlx,1,i)
*d,mh4c.330,mh4c.333                                <25588-25591>
*/ Fix a PVM bug related to counts of detector/DXTRAN large scores.
*d,mh4c.336                                         <25594>
  350 call mputd(ddn(lddn+22,j)-ddn(kddn+22,j),1,i)
*d,mh4c.339                                         <25597>
  360 call mputd(dxd(ldxd+j,22,k)-dxd(kdxd+j,22,k),1,i)
*/ Collect other-side cell data for output/continue-runs. (GWM) 03/12/01
*i,mh4c.350                                         <25608>
      call mputi(laj(llaj+1),(mlaj+mx)*mtasks,i)
      call mputi(lcaj(llcj+1),(mlja+1)*mtasks,i)
*/ Fix cpu timing bugs.                            (GWM) 03/22/01
*i,mh4c.359                                         <25617>
      call mputi(ntc,1,i)
      call mputi(ntc1,1,i)
*d,mh4c.417,mh4c.418                               <25675>-<25676>
      cp3=cp3+t2-t1
      t1=t2
*i,mh4c.421                                         <25679>
      call mputd(cts,1,i)
*ident sp4c3 ----- startp
*/ Print macrobody surfaces in 1st 50 histories.    (JSH) 03/13/01
*d,sp4a.27,sp4a.28                                 <26244>-<26245>
      i=0
      if(jsu.gt.0)i=nsf(lnsf+jsu)
      write(hs,'(i7)')i
      if(i.gt.0.and.i.le.99999.and.kfq.gt.0)write(hs,'(i5,1h.,i1)')i,kfq
*ident aa4c3 ----- avrwwg
*/ Do not use WWG mesh WW values if outside mesh.  (TEB/JAF) 02/08/01
*d,aa4c.21                                         <28285>
      call avrxyz(dc,mi,df,ie)
      if(ie.eq.1)return
*d,aa4c.46                                         <28310>
      50 call avrxyz(cc,mi,df,ie)
      if(ie.eq.1)return
*/ Prevent negative sqrt.                          (TEB/JAF) 02/07/01
*d,aa4c.149                                         <28416>
      dr(1)=-a+sqrt(abs(sq))
*/ Do not use WWG mesh WW values if outside mesh.  (TEB/JAF) 02/08/01
*d,aa4c.200                                         <28469>
      call avrxyz(cc,mi,df,ie)
```

```
*ident aa4c3 ----- avrxyz
*/ Do not use WWG mesh WW values if outside mesh.      (TEB/JAF) 02/08/01
*d,vx4c.2                                              <28489>
      subroutine avrxyz(rc,km,df,no)
*ident rmi4c3 ----- rmcini
*/ Set RMC weight above cutoff if necessary.          (TEB) 01/30/01
*d,rms.124                                             <28654>
      go to 430
      420 continue
      if(wcs1tc(ipt).ne.0)
      1 wgt=wcs1tc(ipt)*fim(lfim+ipt,mai)/fim(lfim+ipt,icl)
      430 continue
*ident ad4c3 ----- addtfc
*/ Fix cpu timing bugs.                                (GWM) 03/22/01
*d,ad.27                                              <39464>
*d,ad4c.5                                             <39484>
      tfc(ltfc+3,1,it)=(cts-cpk)*tfc(ltfc+2,1,it)**2
*ident ay4c3 ----- acalc
*/ PVM bug with acode.                                (GWM) 03/11/01
*/ Incorrect define sequence - should match im4c.33.
*d,ay4c.318                                           <40215>
*if -def,multt.and.multp,3
*d,ay4c.332                                           <40229>
*if -def,multt.and.multp,3
*ident ph4c3 ----- prtfcc
*/ Remove kcode settle time, cpk, from tally signal/noise ratio.
*/ (Rare, when pt=0.)                                 (JSH) 03/21/01
*d,ph4b.34                                             <44259>
      if(pt.eq.0.)pt=60.*nps/max(one,cts-cpk)
*ident vz4c3 ----- avrout
*/ Correct print table 190 print.                     (JSH) 01/31/01
*d,vz4c2.6,vz4c2.11                                  <45020>-<45024>
*i,vz4c.30 after if(c1...)c1=                         <45033>
c
c      write normalization constant for generated mesh windows.
      if(ink(190).ne.0.and.nwgeoa.lt.3)write(iuo,15)ngww(nips),cn,c1
      15 format(35h1mesh-based weight window generator,54x,
      1 15hprint table 190//5x,14hnormalization:,i4,7h-group:,
      2 1p1e12.4,10x,8h1-group:,e12.4//)
*ident mp4c3 ----- comdeck mp
*/ Cannot plot electrons (photoneutron error) XBUG    (RCL/JSH) 02/28/01
*d,mp4b.2                                             <45385>
      3 itfc,itik(2),ititle(7),j3d,jlbl(2,9),jlim(2),kbin(8,2),klbl(43),
*ident zb4c3 ----- block data zbldat
*/ Cannot plot electrons (photoneutron error) XBUG    (RCL/JSH) 02/28/01
```

```
*d,zb4b.22 <45443>
  data jlbl/1,7,1,7,19,19,8,10,11,16,21,28,21,28,0,0,31,43/
*d,zb4b.76 <45497>
c data jlbl/1,7,1,7,19,19,8,10,11,16,21,28,21,28,0,0,31,43/
*ident mq4c3 ----- mreset
*/ Cannot plot electrons (photoneutron error) XBUG (RCL/JSH) 02/28/01
*d,mq4b.24 <46385>
  if(kxspar.eq.3.and.kxsptp.eq.9)kxspmt=3
*ident mw4c3 ----- mctalw
*/ Array overflow for macrobodies on mctal files. XBUG(GWM/JSH) 02/28/01
*d,mw4c2.6 <46496>
  15 if(ksm(lksm+i).ne.0)kq=1
*ident cb4c3 ----- chkxss
*/ Clean up xsec plotting: false warning. (JSH) 03/01/01
*d,cb4b.28 <46977>
  if(kxspar.eq.3)write(jtty,50)
*/ Cannot plot electrons (photoneutron error) XBUG (RCL/JSH) 02/28/01
*d,cb4b.92,cb4b.94 <47041>-<47043>
  if(kxsptp.le.4.or.kxsptp.eq.6)kxspar=1
  if(kxsptp.eq.5.or.kxsptp.eq.7.or.kxsptp.eq.8)kxspar=2
  if(kxsptp.eq.9)kxspar=3
*d,cb4b.97 <47046>
  go to(270,270,270,560,630,430,430,9090,670)kxsptp
*ident av4c3 ----- abvals
*/ Cannot plot electrons (photoneutron error) XBUG (RCL/JSH) 02/28/01
*d,av4b.16 <47991>
  if(kxspar.lt.3.or.kxsptp.ne.9)go to 160
*ident ra4c3 ----- random
*/ Correct setting of dbcn(8) X-5:REP-00-117 (REP/JSH) 09/14/00
*d,ra4c2.1,ra4c2.3 <50857>-<50859>
  k=nint(dbcn(8))
  if(dbcn(20).eq.0..and.dbcn(1).ne.0.)k=k-1
  if(dbcn(29).eq.0.)k=nint(dbcn(8))-1
  do 40 i=1,k
*ident gi4c3 ----- getidt
*/ Provide the F90 time and date call. (GWM) 03/14/01
*/ *d,gi4c.1,gi4a.8 <51216-51247>
*/ call date_and_time(values=it)
*/ write(hi,10)it(2),it(3),it(1)-(it(1)/100)*100,it(5),it(6),it(7)
*/ 10 format(2x,i2.2,1h/,i2.2,1h/,i2.2,1x,i2.2,1h:,i2.2,1h:,i2.2)
```

JSH:jsh

Distribution:

X-5 File

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