Summary of changes

Modifications are shown in green, original code from the repository tristan-mp-pu-master is shown in red. Comments, interspersed throughout, are shown in shaded boxes (comments in red boxes should be read as warnings). The normal diff notation (e.g., 73,74d72, 166,187c163,165, \cdots) indicates the lines compared between the two files, and the action performed (d \rightarrow 'deleted', c \rightarrow 'changed', a \rightarrow 'added'). Each section corresponds to a file in tristan-mp-pu-master, and subsections indicate the modified subroutine or function.

The ghost-cell modifications have been tested in 2D and 3D, for periodic boundaries in x, y, and z. The the user file user_weibel.F90 shows an example of necessary modifications for the Weibel problem, and similar changes would be required for other user files (not implemented).

1 Makefile

Add compile time options to specify current deposit scheme (also the associated mover). Also use the unroll option (I get some modest speedup by unrolling loops; can further customize by specifying the unroll depth, e.g. -unroll=4)

```
26c25

< CUSTOMO= -DMPI -DHDF5 -DserIO -Ddd3 -unroll

---

> CUSTOMO= -DMPI -DHDF5 -DserIO
```

This comment is added to document the different options for current deposit scheme: zigzag, 1st, 2nd, and 3rd order Esirkepov density decomposition.

```
50,53d48
< # -Dzzag use zigzag current deposit
< # -Ddd1 use 1st order density decomposition
< # -Ddd2 use 2nd order density decomposition
< # -Ddd3 use 3rd order density decomposition
```

2 fields.F90

2.1 read_input_grid()

Define two variables nghost and nghostz for the number of ghost cells in the (x, y), and z directions, respectively:

Depending on the choice of current deposit scheme (via compile-time option Dzzag, Ddd1, Ddd2, or Ddd3), set the number of ghost cells. The choice nghost = 7 for the 2^{nd} order current deposit is not the minimum number of cells required for a 2^{nd} order shape function, however we keep with the convention that the number of ghost cells is odd, and in this case more than 5 ghost cells are required. The number of ghost cells at lower boundary is |nghost/2|, and the number of ghost cells at the upper boundary is |nghost/2| + 1.

```
166,187c163,165
< #ifdef zzag
          nghost=5
          nghostz=5
< #endif
< #ifdef dd1
          nghost=5
          nghostz=5
< #endif
< #ifdef dd2
          nghost=7
          nghostz=7
< #endif
< #ifdef dd3
          nghost=7
          nghostz=7
< #endif
```

In 2D, no reference is made to particle shape along the z-direction, so only the default 5 ghost cells are necessary; the Eqs. of [1], Sec. 5, are followed for the reduction to 2D.

```
< #ifdef twoD
< nghostz=5
< #endif</pre>
```

Since tristan-mp-pu-master assumes 5 ghost cells, and the modified code assumes (nghost, nghost, nghostz) ghost cells for the (x,y,z) directions, any hardcoded reference to ghost cells should be changed; this sort of change is common in the remainder of the document, and will generally be listed without comment.

2.2 allocate_fields()

```
237c215
        if(modulo(int(my0-nghost), sizey).ne.0) then
---
        if(modulo(int(my0-5),sizey).ne.0) then
240c218
        if(modulo(int(mz0-nghostz),sizez).ne.0) then
___
        if(modulo(int(mz0-5),sizez).ne.0) then
260,262c238,240
                mx=(mx0-nghost)/sizex+nghost
                my=(my0-nghost)/sizey+nghost
                mz=(mz0-nghostz)/sizez+nghostz
                mx = (mx0-5)/sizex+5
                my=(my0-5)/sizey+5
                mz = (mz0-5)/sizez+5
265c243
                        if(mx0 .ne. (mx-nghost)*sizex+nghost) mx=mx0-(mx-nghost)*(sizex-1)
                        if (mx0 .ne. (mx-5)*sizex+5) mx=mx0-(mx-5)*(sizex-1)
268c246
                        if(my0 .ne. (my-nghost)*sizey+nghost) my=my0-(my-nghost)*(sizey-1)
___
                        if (my0 .ne. (my-5)*sizey+5) my=my0-(my-5)*(sizey-1)
279c257
                        if(mz0 .ne. (mz-nghostz)*sizez+nghostz) mz=mz0-(mz-nghostz)*(sizez-1)
                        if (mz0 .ne. (mz-5)*sizez+5) mz=mz0-(mz-5)*(sizez-1)
299c277,278
                mx0=sum(mxl(i1:i2)-nghost)+nghost
                mx0=sum(mx1(i1:i2)-5)+5
302c281
                my0=sum(myl(j1:j2:sizex)-nghost)+nghost
                my0=sum(myl(j1:j2:sizex)-5)+5
310c289
                mz0=sum(mzl(k1:k2:(sizex*sizey))-nghostz)+nghostz
---
                mz0=sum(mz1(k1:k2:(sizex*sizey))-5)+5
318c297
        mxcum=sum(mxl(i1:i2)-nghost)-(mxl(i2)-nghost)
<
---
        mxcum=sum(mx1(i1:i2)-5)-(mx1(i2)-5)
322c301
<
        mycum=sum(myl(j1:j2:sizex)-nghost)-(myl(j2)-nghost)
___
        mycum=sum(myl(j1:j2:sizex)-5)-(myl(j2)-5)
327c306
        mzcum=sum(mzl(k1:k2:(sizex*sizey))-nghostz)-(mzl(k2)-nghostz)
---
        mzcum=sum(mzl(k1:k2:(sizex*sizey))-5)-(mzl(k2)-5)
```

When using a higher-order shape function, current may be deposited beyond the default 2 (3) ghost cells at the bottom (top) of the domain; 2 ghost cells at the bottom, and 3 at the top is enough for a 1^{st} order shape, but a particle with higher-order shape is wider, and requires more ghost cells (the exact number depends on the particle shape). Because of this, buffers used for the exchange of current must be resized. sendbufy and sendbufz are left unchanged.

```
357,360c336,339
         allocate( bufferin1(mx,my,nghostz/2+1),bufferin2(mx,my,nghostz/2), &
         bufferin1y(mx,nghost/2+1,mz),bufferin2y(mx,nghost/2,mz), &
         bufferin1x(nghost/2+1,my,mz),bufferin2x(nghost/2,my,mz), &
<
         sendbufy(mx,2,mz),sendbufz(mx,my,2))
<
         allocate(bufferin1(mx,my,2),bufferin2(mx,my,2), &
         bufferin1y(mx,2,mz),bufferin2y(mx,2,mz), &
bufferin1x(2,my,mz),bufferin2x(2,my,mz), &
         sendbufy(mx,2,mz),sendbufz(mx,my,2))
365.366c344
        call create_MPI_filter_datatypes(nghost/2+1,mx-(nghost/2+1),nghost/2+1,& my-(nghost/2+1),(nghostz/2+1),mz-(nghostz/2+1))
<
<
         call create_MPI_filter_datatypes(3,mx-3,3,my-3,3,mz-3)
2.3 iloc()
388.389c366.367
< if(iloc < nghost/2+1) iloc=1
< if(iloc > mx-(nghost/2)) iloc=mx
> if(iloc < 3) iloc=1</pre>
> if(iloc > mx-2) iloc=mx
2.4 jloc()
401,402c379,380
< if(jloc < (nghost/2+1)) jloc=1
< if(jloc > my-(nghost/2)) jloc=my
> if(jloc < 3) jloc=1
> if(jloc > my-2) jloc=my
2.5 kloc()
414,415c392,393
< if(kloc < (nghostz/2+1)) kloc=1
< if(kloc > mz-(nghostz/2)) kloc=mz
> if(kloc < 3) kloc=1</pre>
> if(kloc > mz-2) kloc=mz
```

2.6 advance_b_halfstep()

The indices for field advance are modified to extend over physical cells, in the general case $nghost \neq 5$.

```
600,601c578,579
                 i1=nghost/2+1
                 i2=mx-(nghost/2+1)
<
                 i1 = 3
                i2=mx-3
603,604c581,582
                 i1=(nghost/2+1)
<
                 i2=mx-(nghost/2+1)
---
                 i1 = 3
                 i2=mx-3
607c585
                         i2=mx-(nghost/2+1)
---
                         i2 = mx - 3
610c588
                         i1=(nghost/2+1)
---
                         i1=3
621,622c599,600
                 j1=(nghost/2+1)
                 j2=my-(nghost/2+1)
                 j2=my-3
```

```
624,625c602,603
                  j1=(nghost/2+1)
                  j2=my-(nghost/2+1)
                  j1=3
                  j2=my-3
628c606
                           j2=my-(nghost/2+1)
<
                           j2=my-3
631c609
                           j1=(nghost/2+1)
<
645,646c623,624
                           k1=(nghostz/2+1)
k2=mz-(nghostz/2+1)
<
                           k2=mz-3
648,649c626,627
                           k1=(nghostz/2+1)
k2=mz-(nghostz/2+1)
                           k1=3
                           k2=mz-3
652c630
                                    k2=mz-(nghostz/2+1)
                                    k2=mz-3
655c633
                                    k1=(nghostz/2+1)
>
                                    k1=3
```

2.7 advance_e_fullstep()

The indices for field advance are updated, similar to advance_b_halfstep()

```
753,754c725,726
                 i1=(nghost/2+1)
<
                 i2=mx-(nghost/2+1)
                 i1=3
                 i2=mx-3
756,757c728,729
                 i1=(nghost/2+1)
                 i2=mx-(nghost/2+1)
                 i1=3
759,760c731,732
                         i1=(nghost/2)
                         i2=mx-(nghost/2+1)
---
>
                         i1=2
                         i2=mx-3
763c735
                         i1=(nghost/2+1)
---
                         i1=3
767c739
                         i1=(nghost/2)
---
774,775c746,747
                 j1=(nghost/2+1)
                 j2=my-(nghost/2+1)
                 j2=my-3
777,778c749,750
                 j1=(nghost/2+1)
j2=my-(nghost/2+1)
                 j1=3
                 j2=my-3
780,781c752,753
                         j1=(nghost/2)
                         j2=my-(nghost/2+1)
```

```
j1=2
                           j2=my-3
784c756
                           j1=(nghost/2+1)
<
788c760
                           j1=(nghost/2)
<
                           j1=2
799,800c771,772
                           k1=(nghostz/2+1)
                           k2=mz-(nghostz/2+1)
                           k1=3
                           k2=mz-3
802,803c774,775
                           k1=(nghostz/2+1)
k2=mz-(nghostz/2+1)
---
                           k1=3
                           k2=mz-3
805,806c777,778
                                    k1=(nghostz/2)
k2=mz-(nghostz/2+1)
                                    k2=mz-3
809c781
                                    k1=(nghostz/2+1)
---
                                    k1=3
813c785
                                    k1=(nghostz/2)
---
                                    k1=2
818c790
                  k1=(nghostz/2)
                  k1=2
```

2.8 advance_b_halfstep_1D()

We do not test any cases that use the 1D field update routines. Changes have been implemented, but not tested.

```
892,893c864,865
                i1=(nghost/2+1)
                i2=mx-(nghost/2+1)
                i1=3
                i2=mx-3
900,901c872,873
                j1=(nghost/2+1)
                j2=my-(nghost/2+1)
---
>
                j1=3
                j2=my-3
903,904c875,876
                j1=(nghost/2+1)
                j2=my-(nghost/2+1)
---
                j2=my-3
907c879
                         j2=my-(nghost/2+1)
---
                         j2=my-3
910c882
                        j1=(nghost/2+1)
---
920,921c892,893
                k1=(nghostz/2+1)
                k2=mz-(nghostz/2+1)
                k2=mz-3
927c899
                        k2=mz-(nghostz/2+1)
                         k2=mz-3
```

```
930c902 
< k1=(nghostz/2+1) 
--- 
> k1=3
```

2.9 advance_e_fullstep_1D()

```
971,972c943,944
                i1=(nghost/2+1)
                i2=mx-(nghost/2+1)
                i2=mx-3
974c946
                i1=(nghost/2)
979,980c951,952
                j1=(nghost/2+1)
                j2=my-(nghost/2+1)
                j2=my-3
982,983c954,955
                j1=(nghost/2+1)
                j2=my-(nghost/2+1)
                j2=my-3
985,986c957,958
                         j1=(nghost/2)
j2=my-(nghost/2+1)
                         j2=my-3
989c961
                         j1=(nghost/2+1)
                         j1=3
993c965
                         j1=(nghost/2)
                         j1=2
999,1000c971,972
                k1=(nghostz/2+1)
                k2=mz-(nghostz/2+1)
                k1=3
                k2=mz-3
1002,1003c974,975
                k1=(nghostz/2+1)
                k2=mz-(nghostz/2+1)
                k1=3
1005,1006c977,978
                         k1=(nghostz/2)
                         k2=mz-(nghostz/2+1)
                         k2=mz-3
1009c981
                         k1=(nghostz/2+1)
1013c985
                         k1=(nghostz/2)
                         k1=2
```

2.10 advance_b_halfstep_42()

```
i2=mx-2
1068,1069c1040,1041
                j1=nghost/2+1
                j2=my-(nghost/2+1)
                j2=my-3
1071,1072c1043,1044
                j1=(nghost/2)
                 j2=my-(nghost/2)
                j1=2
                  j2=my-2
1075c1047
                          j2=my-(nghost/2+1)
                          j2=my-3
1078c1050
                          j1=nghost/2+1
---
                          j1=3
1082,1083c1054,1055
                          j1=(nghost/2)
                          j2=my-(nghost/2)
                          j1=2
                          j2=my-2
1090,1091c1062,1063
                        k1=(nghostz/2+1)
                        k2=mz-(nghostz/2+1)
                        k1=3
                        k2=mz-3
1093,1094c1065,1066
                        k1=(nghostz/2+1)
                        k2=mz-(nghostz/2+1)
                        k1 = 3
                        k2=mz-3
1097c1069
                          k2=mz-(nghostz/2+1)
___
                          k2=mz-3
1100c1072
                          k1=(nghostz/2+1)
                          k1=3
1104,1105c1076,1077
                          k1=(nghostz/2)
                          k2=mz-(nghostz/2)
```

2.11 advance_e_fullstep_42()

```
1239,1240c1211,1212
                i1=nghost/2+1
                i2=mx-(nghost/2+1)
                i2=mx-3
1242c1214
                i1=(nghost/2+1)
1252,1253c1224,1225
                j1=nghost/2+1
                j2=my-(nghost/2+1)
                j1=3
                j2=my-3
1255c1227
                j1=(nghost/2+1)
                j1=2 +1
1261,1262c1233,1234
                        k1=(nghostz/2+1)
<
                        k2=mz-(nghostz/2+1)
                        k1=3
                        k2=mz-3
1266,1267c1238,1239
                                k1=(nghostz/2+1)
                                k2=mz-(nghostz/2+1)
```

2.12 lambda()

The function lambda() is defined only when using the (undocumented) option DABSORB, which has not been tested with the ghost cell modifications.

```
1636,1639c1609,1612

    gc_x = 1.*(nghost/2+1) + (mx0 - 1.*nghost)/2 !x coord. of psr center
    gc_y = 1.*(nghost/2+1) + (my0 - 1.*nghost)/2
    gc_z = 1.*(nghostz/2+1) + (mz0 - 1.*nghostz)/2
    rabs=(0.9*(gc_x-1.(nghost/2+1)))**2

---

>    gc_x = 3. + (mx0 - 5.)/2 !x coord. of psr center
    gc_y = 3. + (my0 - 5.)/2
    gc_z = 3. + (mz0 - 5.)/2
    rabs=(0.9*(gc_x-3.))**2

1644c1617

    rmax=gc_x - 1.*(nghost/2+1)
---
    rmax=gc_x - 3.
```

3 fieldboundaries.F90

3.1 read_input_boundaries()

Below is a modification that is relevant when periodicx=0, however the ghost cell changes are tested only in the case of periodic boundaries in x, y, and z. Use of the ghost cell modifications and, for example, outflow boundary conditions, would require additional changes and testing (in general, the required changes should be implemented, but it would be worth double checking deposit_particles subroutine in particles_movedeposit.F90 and filter subroutines in optimized_filters.F90; the specific user file would also require appropriate changes).

```
98,99c98,99

< x1in=nghost/2+1 !set the location of planes where particles are removed from simulation, perpendicular to x.

< x2in=mx0-(nghost/2)

---

x1in=3 !set the location of planes where particles are removed from simulation, perpendicular to x.

x2in=mx0-2
```

3.2 bc_b1()

The range of copied layers in the bc_b1 routine is extended to account for higher-order shape functions. Fields in ghost cells are used not only in the field update, but also in the mover routines. With higher-order shape functions, the particle stencil can extend past the first layer of ghost cells, so to compute the correct force on a particle, the field should be copied into any cell over which the particle's stencil extends. For zigzag current deposit, the routine as written below is copying a layer that is not needed, unless we use the highorder field advance. As written below, the copy statements that would be called when using the highorder option are redundant, so they are commented out.

```
197,200c193
                           do iter=1,nghost/2
                              call copy_layrx2_opt(bx,by,bz,mx,my,mz,&
                                   nghost/2+1-iter, mx-(nghost/2+iter), mx-(nghost/2+1)+iter, nghost/2+iter)
                           enddo
                         call copy_layrx2_opt(bx,by,bz,mx,my,mz,2,mx-3,mx-2,3)
202c195
                                 !call copy_layrx2_opt(bx,by,bz,mx,my,mz,1,mx-4,mx-1,4)
                                 call copy_layrx2_opt(bx,by,bz,mx,my,mz,1,mx-4,mx-1,4)
207,210c200
                           do iter=1,nghost/2
                              call copylayrx(bx.by.bz.mx.my.mz.&
                                   nghost/2+1-iter, mx-(nghost/2+iter), mx-(nghost/2+1)+iter, nghost/2+iter)
<
                           enddo
                         call copylayrx(bx,by,bz,mx,my,mz,2,mx-3,mx-2,3)
212c202
<
                                 !call copylayrx(bx,by,bz,mx,my,mz,1,mx-4,mx-1,4)
                                 call copylayrx(bx,by,bz,mx,my,mz,1,mx-4,mx-1,4)
215a206
218,221c209
                           do iter=1,nghost/2
                              call copy_layry1_opt(bx,by,bz,mx,my,mz,&
                                   nghost/2+1-iter,my-(nghost/2+iter),my-(nghost/2+1)+iter,nghost/2+iter)
<
                           enddo
---
                         call copy_layry1_opt(bx,by,bz,mx,my,mz,2,my-3,my-2,3)
223c211
                                 !call copy_layry1_opt(bx,by,bz,mx,my,mz,1,my-4,my-1,4)
---
                                 call copy_layry1_opt(bx,by,bz,mx,my,mz,1,my-4,my-1,4)
226,229c214
                           do iter=1,nghost/2
                              call copy_layry2_opt(bx,by,bz,mx,my,mz,&
                                   {\tt nghost/2+1-iter,my-(nghost/2+iter),my-(nghost/2+1)+iter,nghost/2+iter)}
<
                           enddo
---
                         call copy_layry2_opt(bx,by,bz,mx,my,mz,2,my-3,my-2,3)
231c216
                                  !call copy_layry2_opt(bx,by,bz,mx,my,mz,1,my-4,my-1,4)
___
                                 call copy_layry2_opt(bx,by,bz,mx,my,mz,1,my-4,my-1,4)
236,239c221
                           do iter=1,nghost/2
                              call copylayry(bx,by,bz,mx,my,mz,&
                                   nghost/2+1-iter,my-(nghost/2+iter),my-(nghost/2+1)+iter,nghost/2+iter)
---
                         call copylayry(bx,by,bz,mx,my,mz,2,my-3,my-2,3)
241c223
                                 !call copylayry(bx,by,bz,mx,my,mz,1,my-4,my-1,4)
___
                                 call copylayry(bx,by,bz,mx,my,mz,1,my-4,my-1,4)
244a227
246,249c229
                  do iter=1,nghostz/2
                     call copy_layrz1_opt(bx,by,bz,mx,my,mz,&
                           nghostz/2+1-iter,mz-(nghostz/2+iter),mz-(nghostz/2+1)+iter,nghostz/2+iter)
<
<
                call copy_layrz1_opt(bx,by,bz,mx,my,mz,2,mz-3,mz-2,3)
251c231
                         !call copy_layrz1_opt(bx,by,bz,mx,my,mz,1,mz-4,mz-1,4)
                         call copy_layrz1_opt(bx,by,bz,mx,my,mz,1,mz-4,mz-1,4)
255,258c235
                  do iter=1,nghostz/2
                     call copy_layrz2_opt(bx,by,bz,mx,my,mz,&
    nghostz/2+1-iter,mz-(nghostz/2+iter),mz-(nghostz/2+1)+iter,nghostz/2+iter)
<
<
                  enddo
---
                call copy_layrz2_opt(bx,by,bz,mx,my,mz,2,mz-3,mz-2,3)
260c237
                         ! \verb| call copy_layrz2_opt (bx, by, bz, mx, my, mz, 1, mz-4, mz-1, 4)|\\
                         call copy_layrz2_opt(bx,by,bz,mx,my,mz,1,mz-4,mz-1,4)
262a240
```

3.3 bc_e1()

The changes here are similar to those needed in bc_b1().

```
310,311d287
          integer iter
314,317c290
                           do iter=1,nghost/2
                              call copy_layrx1_opt(ex,ey,ez,mx,my,mz,&
                                   nghost/2+1-iter, mx-(nghost/2+iter), mx-(nghost/2+1)+iter, nghost/2+iter)
<
                           enddo
                         call copy_layrx1_opt(ex,ey,ez,mx,my,mz,2,mx-3,mx-2,3)
319c292
                                 !call copy_layrx1_opt(ex,ey,ez,mx,my,mz,1,mx-4,mx-1,4)
                                 call copy_layrx1_opt(ex,ey,ez,mx,my,mz,1,mx-4,mx-1,4)
322,325c295
                           do iter=1,nghost/2
                              call copy_layrx2_opt(ex,ey,ez,mx,my,mz,&
<
                                   nghost/2+1-iter, mx-(nghost/2+iter), mx-(nghost/2+1)+iter, nghost/2+iter)
                           enddo
---
                         call copy_layrx2_opt(ex,ey,ez,mx,my,mz,2,mx-3,mx-2,3)
327c297
                                 !call copy_layrx2_opt(ex,ey,ez,mx,my,mz,1,mx-4,mx-1,4)
___
                                 call copy_layrx2_opt(ex,ey,ez,mx,my,mz,1,mx-4,mx-1,4)
332,335c302
                           do iter=1,nghost/2
                              call copylayrx(ex,ey,ez,mx,my,mz,&
                                   nghost/2+1-iter,mx-(nghost/2+iter),mx-(nghost/2+1)+iter,nghost/2+iter)
<
---
                         call copylayrx(ex,ey,ez,mx,my,mz,2,mx-3,mx-2,3)
337c304
                                 !call copylayrx(ex,ey,ez,mx,my,mz,1,mx-4,mx-1,4)
                                 call copylayrx(ex,ey,ez,mx,my,mz,1,mx-4,mx-1,4)
344,347c311
                           do iter=1,nghost/2
                              call copy_layry1_opt(ex,ey,ez,mx,my,mz,&
                                   nghost/2+1-iter, my-(nghost/2+iter), my-(nghost/2+1)+iter, nghost/2+iter)
                         call copy_layry1_opt(ex,ey,ez,mx,my,mz,2,my-3,my-2,3)
349c313
                                 !call copy_layry1_opt(ex,ey,ez,mx,my,mz,1,my-4,my-1,4)
                                 \verb|call copy_layry1_opt(ex,ey,ez,mx,my,mz,1,my-4,my-1,4)| \\
352,356c316
                           do iter=1,nghost/2
                              call copy lavry2 opt(ex.ev.ez.mx.mv.mz.&
<
                                   nghost/2+1-iter, my-(nghost/2+iter), my-(nghost/2+1)+iter, nghost/2+iter)
                           enddo
<
                           ! call \ copy_layry2_opt(ex, ey, ez, mx, my, mz, nghost/2-4, my-(nghost/2+5), my-(nghost/2-4), (nghost/2+5)) \\
                         call copy_layry2_opt(ex,ey,ez,mx,my,mz,2,my-3,my-2,3)
358c318
                                 !call copy_layry2_opt(ex,ey,ez,mx,my,mz,1,my-4,my-1,4)
<
---
                                 call copy_layry2_opt(ex,ey,ez,mx,my,mz,1,my-4,my-1,4)
363,366c323
                           do iter=1,nghost/2
<
                              call copylayry(ex,ey,ez,mx,my,mz,&
                                   nghost/2+1-iter,my-(nghost/2+iter),my-(nghost/2+1)+iter,nghost/2+iter)
<
<
                           enddo
---
                         call copylayry(ex,ey,ez,mx,my,mz,2,my-3,my-2,3)
368c325
                                 !\, \verb|call copylayry(ex,ey,ez,mx,my,mz,1,my-4,my-1,4)|\\
---
                                 call copylayry(ex,ey,ez,mx,my,mz,1,my-4,my-1,4)
374.377c331
                  do iter=1,nghostz/2
                      call copy_layrz1_opt(ex,ey,ez,mx,my,mz,&
                           nghostz/2+1-iter,mz-(nghostz/2+iter),mz-(nghostz/2+1)+iter,nghostz/2+iter)
                  enddo
---
                call copy_layrz1_opt(ex,ey,ez,mx,my,mz,2,mz-3,mz-2,3)
379c333
                         ! \verb| call copy_layrz1_opt(ex, ey, ez, mx, my, mz, 1, mz-4, mz-1, 4)|\\
```

3.4 copy_layrz2()

3.5 exchange_current()

The indices for exchange current are generalized to $nghost \neq 5$; also, current from **all** ghost cells is deposited into physical cells (the final ghost cell at the top of the domain is not ignored). Without this change, current that is deposited in the last ghost cell at the top of the domain will be discarded. This change necessitates separate variables count, count2 corresponding to transfer of ghost cells from the top or bottom of the domain, respectively.

```
1774c1725
        integer :: uprank, dwnrank, comm,count,count2,uptag,dwntag,ierr, &
---
        integer :: uprank, dwnrank, comm,count,uptag,dwntag,ierr, &
1798,1811c1748,1761
                bufferin1x(1:nghost/2+1,:,:)=curx((mx-nghost/2):(mx),:,:)
                bufferin2x(1:nghost/2,:,:)=curx(1:nghost/2,:,:)
                curx((nghost/2+1):(nghost),:,:)=curx((nghost/2+1):(nghost),:,:)+bufferin1x(1:nghost/2+1,:,:)
                curx((mx-(nghost-1)):(mx-(nghost/2+1)),:,:)=curx(&
                        (mx-(nghost-1)):(mx-(nghost/2+1)),:,:)+bufferin2x(1:nghost/2,:,:)
                bufferin1x(1:nghost/2+1,:,:)=cury((mx-nghost/2):(mx),:,:)
                bufferin2x(1:nghost/2,:,:)=cury(1:nghost/2,:,:)
                cury((nghost/2+1):(nghost),:,:)=cury((nghost/2+1):(nghost),:,:)+bufferin1x(1:nghost/2+1,:,:)
                cury(mx-(nghost-1):(mx-(nghost/2+1)),:,:)=cury(&
                        mx-(nghost-1):(mx-(nghost/2+1)),:,:)+bufferin2x(1:nghost/2,:,:)
                bufferin1x(1:nghost/2+1,:,:)=curz((mx-nghost/2):(mx),:,:)
                bufferin2x(1:nghost/2,:,:)=curz(1:nghost/2,:,:)
                curz((nghost/2+1):(nghost),:,:)=curz((nghost/2+1):(nghost),:,:)+bufferin1x(1:nghost/2+1,:,:)
                curz((mx-(nghost-1)):(mx-(nghost/2+1)),:,:)=curz(&
<
                        (mx-(nghost-1)):(mx-(nghost/2+1)),:,:)+bufferin2x(1:nghost/2,:,:)
                bufferin1x(1:2,:,:)=curx(mx-2:mx-1,:,:)
                bufferin2x(1:2,:,:)=curx(1:2,:,:)
                curx(3:4,:,:)=curx(3:4,:,:)+bufferin1x(1:2,:,:)
                curx(mx-4:mx-3,:,:)=curx(mx-4:mx-3,:,:)+bufferin2x(1:2,:,:)
                bufferin1x(1:2,:,:)=cury(mx-2:mx-1,:,:)
                bufferin2x(1:2,:,:)=cury(1:2,:,:)
                cury(3:4,:,:)=cury(3:4,:,:)+bufferin1x(1:2,:,:)
                cury(mx-4:mx-3,:,:)=cury(mx-4:mx-3,:,:)+bufferin2x(1:2,:,:)
                bufferin1x(1:2,:,:)=curz(mx-2:mx-1,:,:)
                bufferin2x(1:2,:,:)=curz(1:2,:,:)
                curz(3:4,:,:)=curz(3:4,:,:)+bufferin1x(1:2,:,:)
                curz(mx-4:mx-3,:,:)=curz(mx-4:mx-3,:,:)+bufferin2x(1:2,:,:)
1832,1833c1782
                count=(j2-j1+1)*(nghost/2+1)
                  count2=(j2-j1+1)*(nghost/2)
___
                count = (j2-j1+1)*2
1837,1838c1786
                count = (j2-j1+1)*(k2-k1+1)*(nghost/2+1)
                  count2=(i2-i1+1)*(k2-k1+1)*(nghost/2)
                count = (j2-j1+1)*(k2-k1+1)*2
1841,1842c1789,1790
```

```
call MPI_SendRecv(curx((mx-nghost/2):mx,j1:j2,k1:k2),count,mpi_read,plusrank &
                                                                 ,plustag,bufferin1x(1:nghost/2+1,j1:j2,k1:k2), count,mpi_read,minusrank,plustag, &
                                                                call MPI_SendRecv(curx(mx-2:mx-1, j1: j2,k1:k2),count,mpi_read,plusrank &
                                                                 ,plustag,bufferin1x(1:2,j1:j2,k1:k2), count,mpi_read,minusrank,plustag, &
1847,1850c1795
                                                                if(iperiodic) then
                                                                                         curx((nghost/2+1):(nghost),j1:j2,k1:k2)=curx((nghost/2+1):(nghost),j1:j2,k1:k2)&
                                                                                                            +bufferin1x(1:nghost/2+1,j1:j2,k1:k2)
                                                                        endif
<
                                                                 if(iperiodic) curx(3:4,j1:j2,k1:k2)=curx(3:4,j1:j2,k1:k2)+bufferin1x(1:2,j1:j2,k1:k2)
1854,1855c1799,1800
                                                                call MPI_SendRecv(curx(1:nghost/2,j1:j2,k1:k2),count2,mpi_read,minusrank,minustag, &
                                                                bufferin2x(1:nghost/2,j1:j2,k1:k2),count2,mpi_read,plusrank,minustag, comm &
<
                                                                \verb|call MPI_SendRecv(curx(1:2,j1:j2,k1:k2),count,mpi_read,minusrank,minustag, \& left | left 
                                                                bufferin2x(1:2,j1:j2,k1:k2),count,mpi_read,plusrank,minustag, comm &
1860.1863c1805
                                                                if(iperiodic) then
                                                                                        \verb|curx(mx-(nghost-1):(mx-(nghost/2+1)),j1:j2,k1:k2)| = \verb|curx(mx-(nghost-1):(mx-(nghost/2+1)),j1:j2,k1:k2)| = \verb|curx(mx-(nghost-1):(mx-(nghost-1)),j1:j2,k1:k2)| = \verb|curx(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(n
<
                                                                                                             +bufferin2x(1:nghost/2,j1:j2,k1:k2)
<
                                                                        endif
                                                                1872,1873c1814,1815
                                                                call MPI_SendRecv(cury((mx-nghost/2):mx,j1:j2,k1:k2),count,mpi_read,plusrank &
<
                                                                 \tt ,plustag,bufferin1x(1:nghost/2+1,j1:j2,k1:k2), count,mpi\_read,minusrank,plustag, \& line for the context of 
                                                                call MPI_SendRecv(cury(mx-2:mx-1,j1:j2,k1:k2),count,mpi_read,plusrank &
                                                                   ,plustag,bufferin1x(1:2,j1:j2,k1:k2), count,mpi_read,minusrank,plustag, &
1878,1881c1820,1821
                                                                if(iperiodic) then
                                                                                         +bufferin1x(1:nghost/2+1,j1:j2,k1:k2)
 <
                                                                        endif
                                                                if(iperiodic) cury(3:4,j1:j2,k1:k2)=cury(3:4,j1:j2,k1:k2)+bufferin1x(1:2,j1:j2,k1:k2)
1884,1885c1824,1825
                                                                 \texttt{bufferin2x(1:nghost/2,j1:j2,k1:k2),count2,mpi\_read,plusrank,minustag,~comm~\&~application and application application and a
___
                                                                 call MPI_SendRecv(cury(1:2,j1:j2,k1:k2),count,mpi_read,minusrank,minustag, &
                                                                 bufferin2x(1:2,j1:j2,k1:k2),count,mpi_read,plusrank,minustag, comm &
1890,1893c1830
                                                                 if(iperiodic) then
                                                                                         +bufferin2x(1:nghost/2,j1:j2,k1:k2)
                                                                  if(iperiodic) cury(mx-4:mx-3,j1:j2,k1:k2)=cury(mx-4:mx-3,j1:j2,k1:k2)+bufferin2x(1:2,j1:j2,k1:k2)
1900,1901c1837,1838
                                                                call MPI_SendRecv(curz((mx-nghost/2):(mx),j1:j2,k1:k2),count,mpi_read,plusrank &
                                                                 ,plustag,bufferin1x(1:nghost/2+1,j1:j2,k1:k2), count,mpi_read,minusrank,plustag, &
                                                                call MPI_SendRecv(curz(mx-2:mx-1,j1:j2,k1:k2),count,mpi_read,plusrank &
                                                                 ,plustag,bufferin1x(1:2,j1:j2,k1:k2), count,mpi_read,minusrank,plustag, &
1906,1909c1843
                                                                if (iperiodic) then
                                                                                         curz((nghost/2+1):(nghost), j1:j2,k1:k2)=curz((nghost/2+1):(nghost), j1:j2,k1:k2)&
                                                                                                             +bufferin1x(1:nghost/2+1,j1:j2,k1:k2)
                                                                        endif
 <
                                                                 if(iperiodic) curz(3:4,j1:j2,k1:k2)=curz(3:4,j1:j2,k1:k2)+bufferin1x(1:2,j1:j2,k1:k2)
1913,1914c1847,1848
                                                                 bufferin2x(1:nghost/2,j1:j2,k1:k2),count2,mpi_read,plusrank,minustag, comm &
<
                                                                \verb|call MPI_SendRecv(curz(1:2,j1:j2,k1:k2),count,mpi_read,minusrank,minustag, \& left | \& lef
                                                                bufferin2x(1:2,j1:j2,k1:k2),count,mpi_read,plusrank,minustag, comm &
1919.1922c1853
                                                                if (iperiodic) then
                                                                                         \verb"curz(mx-(nghost-1):(mx-(nghost/2+1)),j1:j2,k1:k2) = \verb"curz(mx-(nghost-1):(mx-(nghost/2+1)),j1:j2,k1:k2) = \verb"curz(mx-(nghost-1):(mx-(nghost/2+1)),j1:j2,k1:k2) = \verb"curz(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost/2+1)),j1:j2,k1:k2) = \verb"curz(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(nghost-1):(mx-(ng
<
                                                                                                            +bufferin2x(1:nghost/2,j1:j2,k1:k2)
<
                                                                        endif
                                                                if(iperiodic) \ curz(mx-4:mx-3,j1:j2,k1:k2) = curz(mx-4:mx-3,j1:j2,k1:k2) + bufferin2x(1:2,j1:j2,k1:k2)
1933,1946c1864,1877
                                                                 bufferin1y(:,1:nghost/2+1,:)=curx(:,(my-(nghost/2)):(my),:)
                                                                bufferin2y(:,1:nghost/2,:)=curx(:,1:nghost/2,:)
<
                                                                 curx(:,(nghost/2+1):(nghost),:)=curx(:,(nghost/2+1):(nghost),:)+bufferin1y(:,1:nghost/2+1,:)
<
                                                                 +bufferin2y(:,1:nghost/2,:)
```

```
bufferin1y(:,1:nghost/2,+1:)=cury(:,(my-(nghost/2)):(my),:)
                bufferin2y(:,1:nghost/2,:)=cury(:,1:nghost/2,:)
               cury(:,(nghost/2+1):(nghost),:)=cury(:,(nghost/2+1):(nghost),:)+bufferin1y(:,1:nghost/2+1,:)
               cury(:,(my-(nghost-1)):(my-(nghost/2+1)),:)=cury(:,(my-(nghost-1)):(my-(nghost/2+1)),:)&
                         +bufferin2y(:,1:nghost/2,:)
                bufferin1y(:,1:nghost/2+1,:)=curz(:,(my-(nghost/2)):(my),:)
               bufferin2y(:,1:nghost/2,:)=curz(:,1:nghost/2,:)
               curz(:,(nghost/2+1):(nghost),:)=curz(:,(nghost/2+1):(nghost),:)+bufferin1y(:,1:nghost/2+1,:)
               curz(:,(my-(nghost-1)):(my-(nghost/2+1)),:) = curz(:,(my-(nghost-1)):(my-(nghost/2+1)),:)&
                        +bufferin2y(:,1:nghost/2,:)
               bufferin1y(:,1:2,:)=curx(:,my-2:my-1,:)
               bufferin2y(:,1:2,:) = curx(:,1:2,:)
curx(:,3:4,:) = curx(:,3:4,:) + bufferin1y(:,1:2,:)
               \verb"curx(:,my-4:my-3,:) = \verb"curx(:,my-4:my-3,:) + \verb"bufferin2y(:,1:2,:)"
               bufferin1y(:,1:2,:)=cury(:,my-2:my-1,:)
bufferin2y(:,1:2,:)=cury(:,1:2,:)
               cury(:,3:4,:)=cury(:,3:4,:)+bufferin1y(:,1:2,:)
               cury(:,my-4:my-3,:)=cury(:,my-4:my-3,:)+bufferin2y(:,1:2,:)
               bufferin1y(:,1:2,:)=curz(:,my-2:my-1,:)
               bufferin2y(:,1:2,:)=curz(:,1:2,:)
               curz(:,3:4,:)=curz(:,3:4,:)+bufferin1y(:,1:2,:)
               curz(:,my-4:my-3,:)=curz(:,my-4:my-3,:)+bufferin2y(:,1:2,:)
1981,1982c1913
               count=(i2-i1+1)*(nghost/2+1)
<
                 count2=(i2-i1+1)*(nghost/2)
---
                count=(i2-i1+1)*2
1986,1987c1917
               count = (i2-i1+1)*(k2-k1+1)*(nghost/2+1)
<
                 count2=(i2-i1+1)*(k2-k1+1)*(nghost/2)
___
                count=(i2-i1+1)*(k2-k1+1)*2
1990,1991c1920,1921
               call MPI_SendRecv(curx(i1:i2,(my-(nghost/2)):(my),k1:k2),count,mpi_read,rgtrank &
                ,rgttag,bufferin1y(i1:i2,1:nghost/2+1,k1:k2), count,mpi_read,lftrank,rgttag, &
___
                ,rgttag,bufferin1y(i1:i2,1:2,k1:k2), count,mpi_read,lftrank,rgttag, &
1997,2000c1927
                if (iperiodic) then
                      curx(i1:i2,(nghost/2+1):(nghost),k1:k2)=curx(i1:i2,(nghost/2+1):(nghost),k1:k2)&
                           +bufferin1y(i1:i2,1:nghost/2+1,k1:k2)
                 endif
                if(iperiodic) curx(i1:i2,3:4,k1:k2)=curx(i1:i2,3:4,k1:k2)+bufferin1y(i1:i2,1:2,k1:k2)
2004,2005c1931,1932
               call MPI_SendRecv(curx(i1:i2,1:nghost/2,k1:k2),count2,mpi_read,lftrank,lfttag, &
               bufferin2y(i1:i2,1:nghost/2,k1:k2),count2,mpi_read,rgtrank,lfttag, comm &
                call MPI_SendRecv(curx(i1:i2,1:2,k1:k2),count,mpi_read,lftrank,lfttag, &
                bufferin2y(i1:i2,1:2,k1:k2),count,mpi_read,rgtrank,lfttag, comm &
2011,2014c1938
               if(iperiodic) then
                     curx(i1:i2,(my-(nghost-1)):(my-(nghost/2+1)),k1:k2)=curx(i1:i2,(my-(nghost-1)):(my-(nghost/2+1)),k1:k2)&
                          +bufferin2y(i1:i2,1:nghost/2,k1:k2)
                 endif
                if(iperiodic) curx(i1:i2,my-4:my-3,k1:k2)=curx(i1:i2,my-4:my-3,k1:k2)+bufferin2y(i1:i2,1:2,k1:k2)
2022,2023c1946,1947
               call MPI_SendRecv(cury(i1:i2,(my-(nghost/2)):(my),k1:k2),count,mpi_read,rgtrank &
                ,rgttag,bufferin1y(i1:i2,1:nghost/2+1,k1:k2), count,mpi_read,lftrank,rgttag, &
<
               rgttag, bufferin1y(i1:i2,1:2,k1:k2), count,mpi_read,lftrank,rgttag, &
2029,2033c1953,1954
               if(iperiodic) then
                     cury(i1:i2,(nghost/2+1):(nghost),k1:k2)=cury(i1:i2,(nghost/2+1):(nghost),k1:k2) &
                           +bufferin1y(i1:i2,1:nghost/2+1,k1:k2)
                   endif
<
               if(iperiodic) curv(i1:i2.3:4.k1:k2)=curv(i1:i2.3:4.k1:k2)+bufferin1v(i1:i2.1:2.k1:k2)
2037,2038c1958,1959
                call MPI_SendRecv(cury(i1:i2,1:nghost/2,k1:k2),count2,mpi_read,lftrank,lfttag, &
               bufferin2y(i1:i2,1:nghost/2,k1:k2),count2,mpi_read,rgtrank,lfttag, comm,status &
               call MPI_SendRecv(cury(i1:i2,1:2,k1:k2),count,mpi_read,lftrank,lfttag, &
                bufferin2y(i1:i2,1:2,k1:k2),count,mpi_read,rgtrank,lfttag, comm,status &
2044,2047c1965
               if(iperiodic) then
```

```
\texttt{cury} \ (\texttt{i1}: \texttt{i2}, (\texttt{my}-(\texttt{nghost}-1)): (\texttt{my}-(\texttt{nghost}/2+1)), \texttt{k1}: \texttt{k2}) = \texttt{cury} \ (\texttt{i1}: \texttt{i2}, (\texttt{my}-(\texttt{nghost}-1)): (\texttt{my}-(\texttt{nghost}/2+1)), \texttt{k1}: \texttt{k2}) \\ \texttt{k2} = \texttt{k2} = \texttt{k2} = \texttt{k2} = \texttt{k3} = \texttt{k2} = \texttt{k3} = \texttt{
                                                                                                 +bufferin2y(i1:i2,1:nghost/2,k1:k2)
                                                          if(iperiodic) cury(i1:i2,my-4:my-3,k1:k2)=cury(i1:i2,my-4:my-3,k1:k2)+bufferin2y(i1:i2,1:2,k1:k2)
2053,2054c1971,1972
                                                         call MPI_SendRecv(curz(i1:i2,(my-(nghost/2)):(my),k1:k2),count,mpi_read,rgtrank &
                                                         ,rgttag,bufferin1y(i1:i2,1:nghost/2+1,k1:k2),count,mpi_read,lftrank,rgttag &
                                                         call MPI_SendRecv(curz(i1:i2,my-2:my-1,k1:k2),count,mpi_read,rgtrank &
                                                         ,rgttag,bufferin1y(i1:i2,1:2,k1:k2),count,mpi_read,lftrank,rgttag &
2060,2063c1978
                                                         if (iperiodic) then
                                                                              curz(i1:i2,(nghost/2+1):(nghost),k1:k2)=curz(i1:i2,(nghost/2+1):(nghost),k1:k2)&
                                                                                                +bufferin1y(i1:i2,1:nghost/2+1,k1:k2)
<
                                                                endif
                                                         if(iperiodic) curz(i1:i2,3:4,k1:k2)=curz(i1:i2,3:4,k1:k2)+bufferin1y(i1:i2,1:2,k1:k2)
2069,2070c1984,1985
                                                         call MPI SendRecv(curz(i1:i2.1:nghost/2.k1:k2).count2.mpi read.lftrank.lfttag. &
                                                         \verb|bufferin2y(i1:i2,1:nghost/2,k1:k2)|, \verb|count2,mpi_read,rgtrank|, \verb|lfttag|, & & \\
<
---
                                                         call MPI_SendRecv(curz(i1:i2,1:2,k1:k2),count,mpi_read,lftrank,lfttag, &
                                                         bufferin2y(i1:i2,1:2,k1:k2),count,mpi_read,rgtrank,lfttag, &
2076.2079c1991
                                                         if (iperiodic) then
                                                                              \verb"curz" (i1:i2,(my-(nghost-1)):(my-(nghost/2+1)),k1:k2) = \verb"curz" (i1:i2,(my-(nghost-1)):(my-(nghost/2+1)),k1:k2) = \verb"curz" (i1:i2,(my-(nghost-1)):(my-(nghost/2+1)),k1:k2) = \verb"curz" (i1:i2,(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1)):(my-(nghost-1))
                                                                                                +bufferin2y(i1:i2,1:nghost/2,k1:k2)
<
                                                                endif
---
                                                         if(iperiodic) curz(i1:i2,my-4:my-3,k1:k2)=curz(i1:i2,my-4:my-3,k1:k2)+bufferin2y(i1:i2,1:2,k1:k2)
2101,2102c2013
                                                         count = (i2-i1+1)*(j2-j1+1)*(nghostz/2+1)
<
                                                               count2=(i2-i1+1)*(j2-j1+1)*(nghostz/2)
---
                                                         count=(i2-i1+1)*(j2-j1+1)*2
2108,2109c2019,2020
                                                         call MPI_SendRecv(curx(i1:i2,j1:j2,mz-(nghostz/2):mz),count,mpi_read,uprank,uptag, &
                                                         bufferin1(i1:i2,j1:j2,1:nghostz/2+1),count,mpi_read,dwnrank,uptag, comm &
___
                                                         \verb|call MPI_SendRecv(curx(i1:i2,j1:j2,mz-2:mz-1),count,mpi_read,uprank,uptag, \& left | \& lef
                                                         bufferin1(i1:i2,j1:j2,1:2),count,mpi_read,dwnrank,uptag, comm &
2114,2117c2025
                                                         if (iperiodic) then
                                                                              \verb"curx(i1:i2,j1:j2,(nghostz/2+1):(nghostz)) = \verb"curx(i1:i2,j1:j2,(nghostz/2+1):(nghostz)) \& (nghostz/2+1) = \verb"curx(i1:i2,j1:j2,(nghostz/2+1):(nghostz)) & (nghostz/2+1) = \verb"curx(i1:i2,j1:j2,(nghostz/2+1):(nghostz)) & (nghostz/2+1) = \verb"curx(i1:i2,j1:j2,(nghostz/2+1):(nghostz)) & (nghostz/2+1) & (nghos
                                                                                                +bufferin1(i1:i2,j1:j2,1:nghostz/2+1)
                                                                endif
                                                         if(iperiodic)curx(i1:i2,j1:j2,3:4)=curx(i1:i2,j1:j2,3:4)+bufferin1(i1:i2,j1:j2,1:2)
 2121,2122c2029,2030
                                                         call MPI_SendRecv(curx(i1:i2,j1:j2,1:nghostz/2),count2,mpi_read,dwnrank,dwntag, &
                                                         bufferin2(i1:i2,j1:j2,1:nghostz/2),count2,mpi_read,uprank,dwntag, comm,status &
                                                         call MPI_SendRecv(curx(i1:i2,j1:j2,1:2),count,mpi_read,dwnrank,dwntag, &
                                                         bufferin2(i1:i2,j1:j2,1:2),count,mpi_read,uprank,dwntag, comm,status &
2127,2130c2035,2036
                                                         if(iperiodic) then
                                                                              curx(i1:i2,j1:j2,(mz-(nghostz-1)):(mz-(nghostz/2+1)))=curx(i1:i2,j1:j2,&
                                                                                                (mz-(nghostz-1)):(mz-(nghostz/2+1)))+bufferin2(i1:i2,j1:j2,1:nghostz/2)
                                                                   endif
                                                         if(iperiodic) curx(i1:i2,j1:j2,mz-4:mz-3)=curx(i1:i2,j1:j2,mz-4:mz-3)+bufferin2(i1:i2,j1:j2,1:2)
2135,2136c2041,2042
                                                         call MPI_SendRecv(cury(i1:i2,j1:j2,mz-(nghostz/2):mz),count,mpi_read,uprank,uptag, &
                                                         bufferin1(i1:i2,j1:j2,1:(nghostz/2+1)), count,mpi_read,dwnrank,uptag, comm,status &
                                                         call MPI_SendRecv(cury(i1:i2,j1:j2,mz-2:mz-1),count,mpi_read,uprank,uptag, &
                                                         bufferin1(i1:i2,j1:j2,1:2), count,mpi_read,dwnrank,uptag, comm,status &
2141,2144c2047
                                                         if(iperiodic) then
                                                                              cury(i1:i2,j1:j2,(nghostz/2+1):(nghostz))=cury(i1:i2,j1:j2,(nghostz/2+1):nghostz) &
                                                                                                +bufferin1(i1:i2, j1:j2,1:(nghostz/2+1))
                                                                   endif
<
                                                         if(iperiodic)cury(i1:i2,j1:j2,3:4)=cury(i1:i2,j1:j2,3:4)+bufferin1(i1:i2,j1:j2,1:2)
2148,2149c2051,2052
                                                         call MPI_SendRecv(cury(i1:i2,j1:j2,1:(nghostz/2)),count2,mpi_read,dwnrank,dwntag, &
                                                         call MPI_SendRecv(cury(i1:i2,j1:j2,1:2),count,mpi_read,dwnrank,dwntag, &
                                                         bufferin2(i1:i2,j1:j2,1:2),count,mpi_read,uprank,dwntag, comm,status
2154,2157c2057
                                                                if(iperiodic) then
                                                                            cury(i1:i2,j1:j2,mz-(nghostz-1):mz-(nghostz/2+1))=cury(i1:i2,j1:j2,mz-(nghostz-1):mz-(nghostz/2+1)) &
```

```
+bufferin2(i1:i2,j1:j2,1:nghostz/2)
                                              endif
                                         if(iperiodic) cury(i1:i2,j1:j2,mz-4:mz-3)=cury(i1:i2,j1:j2,mz-4:mz-3)+bufferin2(i1:i2,j1:j2,1:2)
2163,2164c2063,2064
                                         call MPI_SendRecv(curz(i1:i2,j1:j2,mz-(nghostz/2):mz),count,mpi_read,uprank,uptag, &
                                         bufferin1(i1:i2,j1:j2,1:(nghostz/2+1)),count,mpi_read,dwnrank,uptag, &
                                         call MPI_SendRecv(curz(i1:i2,j1:j2,mz-2:mz-1),count,mpi_read,uprank,uptag, &
                                         {\tt bufferin1(i1:i2,j1:j2,1:2),count,mpi\_read,dwnrank,uptag, \&}
2169,2172c2069
                                         if(iperiodic) then
                                                        curz(i1:i2,j1:j2,(nghostz/2+1):nghostz)=curz(i1:i2,j1:j2,(nghostz/2+1):nghostz) &
                                                                     +bufferin1(i1:i2,j1:j2,1:(nghostz/2+1))
<
                                              endif
                                         if(iperiodic)curz(i1:i2,j1:j2,3:4)=curz(i1:i2,j1:j2,3:4)+bufferin1(i1:i2,j1:j2,1:2)
2176.2177c2073.2074
                                         call MPI_SendRecv(curz(i1:i2,j1:j2,1:nghostz/2),count2,mpi_read,dwnrank,dwntag, &
<
                                         bufferin2(i1:i2,j1:j2,1:nghostz/2),count2,mpi_read,uprank,dwntag, &
                                         call MPI_SendRecv(curz(i1:i2,j1:j2,1:2),count,mpi_read,dwnrank,dwntag, &
                                         bufferin2(i1:i2,j1:j2,1:2),count,mpi_read,uprank,dwntag, &
2182,2185c2079
                                         if(iperiodic) then
                                                        \verb"curz" (i1:i2,j1:j2,mz-(nghostz-1):mz-(nghostz/2+1)) = \verb"curz" (i1:i2,j1:j2,mz-(nghostz-1):mz-(nghostz/2+1)) \& (i1:i2,j1:j2,mz-(nghostz-1):mz-(nghostz/2+1)) & (i1:i2,j1:j2,mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz/2+1)) & (i1:i2,j1:j2,mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(nghostz-1):mz-(ngho
                                                                     +bufferin2(i1:i2,j1:j2,1:nghostz/2)
                                              endif
                                          if (iperiodic) \ curz (i1:i2,j1:j2,mz-4:mz-3) = curz (i1:i2,j1:j2,mz-4:mz-3) + bufferin2 (i1:i2,j1:j2,1:2) \\
```

3.6 apply_filter1_opt()

The indices for filter1 are changed to extend over physical cells, in the general case $nghost \neq 5$.

```
2533,2534c2427,2428
        istr=nghost/2 +1
<
        ifin=mx-1 -(nghost/2)
        istr=2 +1
        ifin=mx-1-2
2566,2567c2460,2461
< !
                         call copy_layrx1(curx,cury,curz,mx,my,mz,nghost/2,mx-(nghost/2+1),mx-nghost/2,nghost/2+1)
<
                        \verb|call copy_layrx1_opt(curx,cury,curz,mx,my,mz,nghost/2,mx-(nghost/2+1),mx-nghost/2,nghost/2+1||
> !
                         call copy_layrx1(curx,cury,curz,mx,my,mz,2,mx-3,mx-2,3)
                         call copy_layrx1_opt(curx,cury,curz,mx,my,mz,2,mx-3,mx-2,3)
2569,2570c2463,2464
                         call copy_layrx2(curx,cury,curz,mx,my,mz,nghost/2,mx-(nghost/2+1),mx-nghost/2,nghost/2+1)
<
                        call copy_layrx2_opt(curx,cury,curz,mx,my,mz,nghost/2,mx-(nghost/2+1),mx-nghost/2,nghost/2+1)
> !
                         call copy_layrx2(curx,cury,curz,mx,my,mz,2,mx-3,mx-2,3)
                         call copy_layrx2_opt(curx,cury,curz,mx,my,mz,2,mx-3,mx-2,3)
2575c2469
                do k=(nghostz/2+1),mz-(nghostz/2+1)
___
                do k=3, mz-3
2579c2473
                        do j=(nghost/2+1),my-(nghost/2+1)
---
                        do j=3, my-3
2587c2481
                do k=(nghostz/2+1),mz-(nghostz/2+1)
___
2591c2485
                        do j=(nghost/2+1),my-(nghost/2+1)
---
                        do j=3, my-3
2602c2496
                do k=(nghostz/2+1),mz-(nghostz/2+1)
                do k=3, mz-3
2606c2500
                        do j=(nghost/2+1), my-(nghost/2+1)
                        do j=3, my-3
2614c2508
                do k=(nghostz/2+1),mz-(nghostz/2+1)
                do k=3.mz-3
```

```
2618c2512
                            do j=(nghost/2+1), my-(nghost/2+1)
---
                            do j=3, my-3
2626c2520
                   do k=(nghostz/2+1),mz-(nghostz/2+1)
___
                   do k=3, mz-3
2630c2524
                            do j=(nghost/2+1), my-(nghost/2+1)
                            do j=3, my-3
2638c2532
                   do k=(nghostz/2+1),mz-(nghostz/2+1)
                   do k=3.mz-3
2642c2536
                            do j=(nghost/2+1), my-(nghost/2+1)
                            do j=3,my-3
2652,2653c2546,2547
                            call copy_layry1(curx,cury,curz,mx,my,mz,nghost/2,my-(nghost/2+1),my-(nghost/2),nghost/2+1)
call copy_layry1_opt(curx,cury,curz,mx,my,mz,nghost/2,my-(nghost/2+1),my-(nghost/2),nghost/2+1)
< !
<
---
> !
                            call copy_layry1(curx,cury,curz,mx,my,mz,2,my-3,my-2,3)
                            call copy_layry1_opt(curx,cury,curz,mx,my,mz,2,my-3,my-2,3)
2655,2656c2549,2550
                            call copy_layry2(curx,cury,curz,mx,my,mz,nghost/2,my-(nghost/2+1),my-(nghost/2),nghost/2+1)
call copy_layry2_opt(curx,cury,curz,mx,my,mz,nghost/2,my-(nghost/2+1),my-(nghost/2),nghost/2+1)
< !
<
---
> !
                            \verb|call copy_layry2(curx, cury, curz, mx, my, mz, 2, my-3, my-2, 3)|\\
                            \verb|call copy_layry2_opt(curx, cury, curz, mx, my, mz, 2, my-3, my-2, 3)|\\
2660c2554
                   do k=(nghostz/2+1),mz-(nghostz/2+1)
___
                   do k=3.mz-3
2664c2558
                            do j=(nghost/2+1), my-(nghost/2+1)
---
                            do j=3, my-3
2672c2566
                   do k=(nghostz/2+1),mz-(nghostz/2+1)
___
                   do k=3, mz-3
2676c2570
                            do j=(nghost/2+1), my-(nghost/2+1)
---
                            do j=3, my-3
2684c2578
                   do k=(nghostz/2+1),mz-(nghostz/2+1)
                   do k=3, mz-3
2688c2582
                            do j=(nghost/2+1),my-(nghost/2+1)
                            do j=3, my-3
2696c2590
                   do k=(nghostz/2+1),mz-(nghostz/2+1)
                   do k=3, mz-3
2700c2594
                            do j=(nghost/2+1), my-(nghost/2+1)
                            do j=3, my-3
2708c2602
                   do k=(nghostz/2+1),mz-(nghostz/2+1)
                   do k=3.mz-3
2712c2606
                            do j=(nghost/2+1),my-(nghost/2+1)
---
                            do j=3, my-3
2720c2614
                   do k=(nghostz/2+1),mz-(nghostz/2+1)
---
                   do k=3.mz-3
2724c2618
                            do j=(nghost/2+1), my-(nghost/2+1)
---
                            do j=3, my-3
```

The eighth and ninth arguments of $copy_layrz1_opt$ look like a typo in $apply_filter1_opt()$ of tristan-mp-pu-master (at least the version we're using: see 2735,2736c2629 directly below). It is only called in 3D when using filter1 and periodicz = 1, but potentially a problem. This is updated in the modified version.

```
2735,2736c2629
                                  call copy_layrz1_opt(curx,cury,curz,mx,my,mz,nghostz/2,&
<
                                                        mz-(nghostz/2+1),mz-(nghostz/2),nghostz/2+1)
                                  call copy_layrz1_opt(curx,cury,curz,mx,my,mz,2,my-3,my-2,3)
2740c2633
                                 call copy_layrz2_opt(curx,cury,curz,mx,my,mz,(nghostz/2),&
<
                                                        mz-(nghostz/2+1),mz-(nghostz/2),(nghostz/2+1))
                                 call copy_layrz2_opt(curx,cury,curz,mx,my,mz,2,mz-3,mz-2,3)
2743,2744c2636,2637
                        do k=(nghostz/2+1),mz-(nghostz/2+1)
                                 do j=(nghost/2+1), my-(nghost/2+1)
                        do k=3.mz-3
                                 do j=3,my-3
2751,2752c2644,2645
                        do k=(nghostz/2+1),mz-(nghostz/2+1)
                                 do j=(nghost/2+1), my-(nghost/2+1)
                        do k=3, mz-3
                                 do j=3,my-3
2759,2760c2652,2653
                        do k=(nghostz/2+1),mz-(nghostz/2+1)
                                do j=(nghost/2+1), my-(nghost/2+1)
                        do k=3, mz-3
                                 do j=3, my-3
2767,2768c2660,2661
                        do k=(nghostz/2+1),mz-(nghostz/2+1)
                                 do j=(nghost/2+1), my-(nghost/2+1)
                        do k=3,mz-3
                                 do j=3, my-3
2775,2776c2668,2669
                        do k=(nghostz/2+1),mz-(nghostz/2+1)
                                do j=(nghost/2+1), my-(nghost/2+1)
                        do k=3, mz-3
                                 do j=3,my-3
2783,2784c2676,2677
                        do k=(nghostz/2+1),mz-(nghostz/2+1)
                                 do j=(nghost/2+1), my-(nghost/2+1)
                        do k=3, mz-3
                                 do j=3, my-3
2796c2689
                                 do j=(nghost/2+1), my-(nghost/2+1)
                                 do j=3, my-3
2804c2697
                                 do j=(nghost/2+1), my-(nghost/2+1)
<
---
                                 do j=3, my-3
2812c2705
                                 do j=(nghost/2+1), my-(nghost/2+1)
                                 do j=3, my-3
```

4 domain.F90

As stated previously, we have tested only cases with periodic boundary conditions. The modifications to enlarge_domain_with_disk(), enlarge_ydomain_with_disk() should not be used without further testing.

4.1 enlarge_domain_with_disk()

```
buffsize = max(3*int(ppc0*upsamp_e*c*max((mx-nghost),(my-nghost))),60000)
                 buffsize = max(3*int(ppc0*upsamp_e*c*max((mx-5),(my-5))),60000)
234,242c234,242
                write(7)(((bx(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
                 (((by(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
                 (((bz(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
                 (((ex(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
<
                 (((ey(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
                (((ez(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
(((curx(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
                 (((cury(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
<
                 (((curz(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz)
<
                 write(7)(((bx(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                 (((by(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                 (((bz(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                 (((ex(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                 (((ey(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                 (((ez(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), \&
                 (((curx(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                 (((cury(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                 (((curz(i,j,k),i=1,mxold-3),j=1,my),k=1,mz)
263,265c263
        call create_MPI_filter_datatypes(nghost/2+1,mx-(nghost/2+1), &
<
                                             nghost/2+1, my-(nghost/2+1),&
                                             nghostz/2+1,mz-(nghostz/2+1))
---
        call create_MPI_filter_datatypes(3,mx-3,3,my-3,3,mz-3)
271,272c269,270
                          mz),bufferin1(mx,my,nghostz/2+1),bufferin2(mx,my,nghostz/2),&
                         bufferin1y(mx,nghost/2+1,mz),bufferin2y(mx,nghost/2,mz))
---
>
                         ,mz),bufferin1(mx,my,2),bufferin2(mx,my,2), &
                         bufferin1y(mx,2,mz),bufferin2y(mx,2,mz))
275 c 273
                 allocate(bufferin1x(nghost/2+1,my,mz),bufferin2x(nghost/2,my,mz))
---
                 allocate(bufferin1x(2,my,mz),bufferin2x(2,my,mz))
326,334c324,332
                \verb"read"(7)"(((bx(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), \& \\
                         (((by(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
                         (((bz(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
                         (((ex(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
                         (((ey(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
                         (((ez(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
                         (((curx(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
                         (((cury(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz), &
                         (((curz(i,j,k),i=1,mxold-(nghost/2+1)),j=1,my),k=1,mz)
                read(7)(((bx(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                         (((by(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                         (((bz(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                         (((ex(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                         (((ey(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                         (((ez(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                         (((curx(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                         (((cury(i,j,k),i=1,mxold-3),j=1,my),k=1,mz), &
                         (((curz(i,j,k),i=1,mxold-3),j=1,my),k=1,mz)
357c355
<
                mx0=sum(mx1(i1:i2)-nghost)+nghost
                mx0=sum(mxl(i1:i2)-5)+5
361c359
                mxcum=sum(mxl(i1:i2)-nghost)-(mxl(rank+1)-nghost)
<
                mxcum=sum(mxl(i1:i2)-5)-(mxl(rank+1)-5)
4.2 enlarge_ydomain_with_disk()
405c403
                buffsize = max(10*int(ppc0*c*max((mx-nghost)*(my-nghost),1*(mx-nghost)*(mz-nghostz))) &
---
                buffsize = max(10*int(ppc0*c*max((mx-5)*(my-5),1*(mx-5)*(mz-5)))) &
410c408
                buffsize = max(3*int(ppc0*c*max((mx-nghost),(my-nghost))),60000)
                buffsize = max(3*int(ppc0*c*max((mx-5),(my-5))),60000)
425.433c423.431
                \label{eq:continuous} \mbox{(((by(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), \& }
                 (((bz(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), &
                 (((ex(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), &
<
                 (((\texttt{ey}(\texttt{i},\texttt{j},\texttt{k}),\texttt{i=1},\texttt{mx}),\texttt{j=1},\texttt{myold-(nghost/2+1)}),\texttt{k=1},\texttt{mz}), \ \& \\
                 (((ez(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), &
<
```

```
(((curx(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), &
                 (((cury(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), &
                 (((curz(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz)
                 write(7)(((bx(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                 (((by(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                 (((bz(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                 (((ex(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                 (((ey(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                 (((ez(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
(((curx(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                 (((cury(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
(((curz(i,j,k),i=1,mx),j=1,myold-3),k=1,mz)
457,459c455
        call create_MPI_filter_datatypes(nghost/2+1,mx-(nghost/2+1),&
                                             (nghost/2+1),my-(nghost/2+1),&
                                             (nghostz/2+1),mz-(nghostz/2+1))
        call create_MPI_filter_datatypes(3,mx-3,3,my-3,3,mz-3)
464,465c460,461
                          ,mz),bufferin1(mx,my,nghostz/2+1),bufferin2(mx,my,nghostz/2), &
                         bufferin1y(mx,nghost/2+1,mz),bufferin2y(mx,nghost/2,mz))
                          ,mz),bufferin1(mx,my,2),bufferin2(mx,my,2), &
                         bufferin1y(mx,2,mz),bufferin2y(mx,2,mz))
469c465
                 allocate(bufferin1x(nghost/2+1,my,mz),bufferin2x(nghost/2,my,mz))
---
                 allocate(bufferin1x(2,my,mz),bufferin2x(2,my,mz))
509.517c505.513
                 \verb"read"(7)"(((bx(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), \& \\
                          (((\texttt{by(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), \ \& \\
                          (((bz(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), &
                          (((ex(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), &
<
<
                          (((ey(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), &
                          (((ez(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), &
<
                          (((curx(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), &
<
                          (((cury(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz), \&
                          (((curz(i,j,k),i=1,mx),j=1,myold-(nghost/2+1)),k=1,mz)
___
                 \verb"read"(7)"(((bx(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), \&
                          (((by(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                          (((bz(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                          (((ex(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                          (((ey(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                          (((ez(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                          (((curx(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                          (((cury(i,j,k),i=1,mx),j=1,myold-3),k=1,mz), &
                          (((curz(i,j,k),i=1,mx),j=1,myold-3),k=1,mz)
539c535
                 my0=sum(my1(j1:j2:sizex)-nghost)+nghost
                 my0=sum(myl(j1:j2:sizex)-5)+5
543c539
                 mycum=sum(myl(j1:j2:sizex)-nghost)-(myl(j2)-nghost)
                 mycum=sum(myl(j1:j2:sizex)-5)-(myl(j2)-5)
    particles.F90
69,71d68
          real(sprec) :: three, two, thhalf, nineighth, one, threeq, twoth, half, &
                third, quart, sixth, negsixth, negone
137,138c134
<
          public :: reorder_particles, exchange_particles, zigzag,&
<
                             densdecomp_lord, densdecomp_2ord, densdecomp_3ord, &
---
          public :: reorder_particles, exchange_particles, zigzag, &
169,171c165
                           movwinoffset, pi, external_fields, user_part_bcs, &
<
                              three, two, thhalf, nineighth, one, threeq, twoth, half, &
<
                              third, quart, sixth, negsixth, negone
```

5.1 read_input_particles()

These are a few constants that are precomputed for use in shape function definitions.

movwinoffset, pi, external_fields, user_part_bcs

```
239,252d232 < three=3.
```

```
< two=2.
< thhalf=3/2.
< nineighth=9/8.
< one=1.
< threeq=3/4.
< twoth=2/3.
< half=1/2.
< third=1/3.
< quart=1/4.
< sixth=1/6.
< negsixth=-1/6.
< negone=-1.</pre>
```

5.2 allocate_particles()

```
309c289
           \texttt{buffsize} = \texttt{max}(10*\texttt{int}(\texttt{ppc0*max}(\texttt{upsamp\_e}, \texttt{upsamp\_i})*\texttt{c*max}((\texttt{mx-nghost})*(\texttt{my-nghost}), 1*(\texttt{mx-nghost})*(\texttt{mz-nghost}))), 10000)
<
---
           \texttt{buffsize} = \texttt{max}(10*\texttt{int}(\texttt{ppc0*max}(\texttt{upsamp\_e}, \texttt{upsamp\_i})*\texttt{c*max}((\texttt{mx-5})*(\texttt{my-5}), 1*(\texttt{mx-5})*(\texttt{mz-5}))), 10000)
312c292
<
---
           buffsize = max(3*int(ppc0*max(upsamp_e,upsamp_i)*c*max((mx-nghost),(my-nghost))),1060000)
          \texttt{buffsize = max(3*int(ppc0*max(upsamp_e,upsamp_i)*c*max((mx-5),(my-5))),1060000)}
339,344c319,324
          x1in=1.*(nghost/2+1)
          x2in=mx0-1.*(nghost/2)
          y1in=1.*(nghost/2+1)
<
          y2in=my0-1.*(nghost/2)
          z1in=1.*(nghostz/2+1)
<
          z2in=mz0-1.*(nghostz/2)
          x1in=3.
          x2in=mx0-2.
          y1in=3.
          y2in=my0-2.
          z1in=3.
          z2in=mz0-2.
```

The following subroutines (densdecomp_1ord, densdecomp_2ord, densdecomp_3ord) are implementations of the Esirkepov current deposit algorithm for 1^{st} , 2^{nd} , and 3^{rd} order shape functions [1]. A different subroutine (densdecomp_1ord, densdecomp_2ord, densdecomp_3ord) is used for each choice of shape function; apart from shape function definition, the routines are the same. These are written for speed, not readability. A more readable (also slow) version of the current deposit is copied below (just the key parts, for 3D). The 2D Eqs. are similar, however the weights wx, yy, zy, as well as the z-current update vis-à-vis tzy admit a reduced form, given in Sec. 5 of [1].

```
! 3d not optimized
do iter=1,6
   DSx(iter)=Sx2(iter)-Sx1(iter)
   DSy(iter)=Sy2(iter)-Sy1(iter)
   DSz(iter)=Sz2(iter)-Sz1(iter)
enddo
do iter2=1.6
   do iter1=1,6
      do iter=1.6
          Wx(iter,iter1,iter2)=DSx(iter )*(Sy1(iter1)*Sz1(iter2)+half*DSy(iter1)*Sz1(iter2) &
               +half*Sy1(iter1)*DSz(iter2)+third*DSy(iter1)*DSz(iter2))
          Wy(iter,iter1,iter2)=DSy(iter1)*(Sx1(iter)*Sz1(iter2)+half*DSx(iter)*Sz1(iter2) &
               +half*Sx1(iter )*DSz(iter2)+third*DSx(iter )*DSz(iter2))
          Wz(iter,iter1,iter2)=DSz(iter2)*(Sx1(iter )*Sy1(iter1)+half*DSx(iter )*Sy1(iter1) &
               +half*Sx1(iter )*DSy(iter1)+third*DSx(iter )*DSy(iter1))
      enddo
   enddo
enddo
   do iter=1.6
      do iter1=1,6
         do iter2=1,6
             if(iter.eq.1) then
                tmpx(iter,iter1,iter2)=q*Wx(iter, iter1, iter2)
             else
                tmpx(iter,iter1,iter2)=tmpx(iter-1,iter1,iter2) &
                      + q*Wx(iter,iter1,iter2)
             endif
          enddo
      enddo
   enddo
   do iter=1,6
      do iter1=1,6
         do iter2=1.6
             if(iter1.eq.1) then
                tmpy(iter,iter1,iter2)=q*Wy(iter,iter1,iter2)
             else
                tmpy(iter,iter1,iter2)=tmpy(iter,iter1-1,iter2) &
                      + q*Wy(iter,iter1,iter2)
             endif
          enddo
      enddo
   enddo
   do iter=1,6
      do iter1=1,6
          do iter2=1,6
             if(iter2.eq.1) then
                 tmpz(iter,iter1,iter2)=q*Wz(iter,iter1,iter2)
             else
                tmpz(iter,iter1,iter2)=tmpz(iter,iter1,iter2-1) &
                      + q*Wz(iter,iter1,iter2)
             endif
          enddo
      enddo
   enddo
do iter=1.6
   do iter1=1,6
      do iter2=1.6
          curx(i1-3+iter,j1-3+iter1,k1-3+iter2)=curx(i1-3+iter,j1-3+iter1,k1-3+iter2)+tmpx(iter,iter1,iter2)
          \texttt{cury}(\texttt{i1}-3+\texttt{iter},\texttt{j1}-3+\texttt{iter1},\texttt{k1}-3+\texttt{iter2}) = \texttt{cury}(\texttt{i1}-3+\texttt{iter},\texttt{j1}-3+\texttt{iter1},\texttt{k1}-3+\texttt{iter2}) + \texttt{tmpy}(\texttt{iter},\texttt{iter1},\texttt{iter2})
          curz(i1-3+iter,j1-3+iter1,k1-3+iter2)=curz(i1-3+iter,j1-3+iter1,k1-3+iter2)+tmpz(iter,iter1,iter2)
      enddo
   enddo
enddo
```

5.3 densdecomp_1ord()

```
672,1362d650
                                                  subroutine densdecomp()
< 1
\boldsymbol{<} ! Charge (current) deposition on the grid, Esirkepov algorithm
< subroutine densdecomp_lord(x2,y2,z2,x1,y1,z1,in)
   implicit none
   ! dummy variables
   logical :: in
   real(sprec), intent(in) :: x1,x2
real(sprec), intent(in) :: y1,y2,z1,z2
   real(sprec) :: dx1,dy1,dx2,dy2,dz1,dz2,deltaz
   ! local variables
    real(sprec), DIMENSION(6)::Sx1,Sy1,Sx2,Sy2,Sz1,Sz2
   real(sprec)::curx_add,curx_add_prev,curz_add
    real(sprec), DIMENSION(6)::cury_adds, cury_add_prevs
    real(sprec), DIMENSION(6,6)::curz_adds,curz_add_prevs
    integer::i1,i2,j1,j2,k1,k2,iter,iter1,iter2, &
        iterx1min, iterx1max, itery1min, itery1max, iterz1min, iterz1max,&
         iterx2min,iterx2max,itery2min,itery2max,iterz2min,iterz2max,&
        iterxmin, iterxmax, iterymin, iterymax, iterzmin, iterzmax, &
        i,j,shifti,shiftj,shiftk,12
   i1=aint(x1)
   i2=aint(x2)
   j1=aint(y1)
   i2=aint(v2)
   k1=aint(z1)
   k2=aint(z2)
   shifti=aint(x2)-aint(x1)
   shiftj=aint(y2)-aint(y1)
   shiftk=aint(z2)-aint(z1)
   dx1=x1-aint(x1)
   dy1=y1-aint(y1)
   dx2=x2-aint(x2)
   dy2=y2-aint(y2)
   dz1=z1-aint(z1)
   dz2=z2-aint(z2)
   deltaz=z2-z1
   Sx1(:)=0.
   Sx2(:)=0.
   Sy1(:)=0.
   Sy2(:)=0.
< #ifndef twoD</pre>
< Sz1(:)=0.
   Sz2(:)=0.
   curz_adds=0.
   curz_add_prevs=0.
< #else
< k1=1
< k2=1
   shiftk=0
   curz_add=0.
< #endif
< ! O order form factor
< Sx1(3)=1.-dx1
   Sx1(4)=dx1
   iterx1min = 3
   iterx1max = 4
   Sx2(3+shifti)=1.-dx2
   Sx2(4+shifti)=dx2
   iterx2min=3+shifti
   iterx2max=4+shifti
   Sy1(3)=1.-dy1
   Sy1(4) = dy1
    itery1min = 3
   itery1max = 4
    Sy2(3+shiftj)=1.-dy2
    Sy2(4+shiftj)=dy2
    itery2min=3+shiftj
```

```
itery2max=4+shiftj
   iterxmin=min(iterx1min,iterx2min)
   iterxmax=max(iterx1max,iterx2max)
   iterymin=min(itery1min,itery2min)
   iterymax=max(itery1max,itery2max)
< #ifndef twoD</pre>
  Sz1(3)=1.-dz1
   Sz1(4)=dz1
   iterz1min = 3
   iterz1max = 4
   Sz2(3+shiftk)=1.-dz2
   Sz2(4+shiftk)=dz2
   iterz2min=3+shiftk
   iterz2max=4+shiftk
   iterzmin=min(iterz1min.iterz2min)
   iterzmax=max(iterz1max.iterz2max)
< #endif
< #ifndef twoD
   do iter2=iterzmin,iterzmax
      do iter1=iterymin,iterymax
          do iter=iterxmin,iterxmax
             12=(i1-3+iter)+(j1-3+iter1-1)*iy+(k1-3+iter2-1)*iz
             !if(12.1t.1 .or. 12.gt.lot) then
             ! print *,"lot=",lot,"l2=",l2
! print *,"i1, j1, k1",i1,j1,k1
                 print *,"ix,iy,iz",ix,iy,iz
print *,"iter,iter1,iter2",iter,iter1,iter2
                 print *,"index err"
             !endif
             curx_add=q*((Sx2(iter )-Sx1(iter ))&
                   *(Sy1(iter1)*Sz1(iter2)+half*(Sy2(iter1)-Sy1(iter1))*Sz1(iter2)\&
                   +half*Sy1(iter1)*(Sz2(iter2)-Sz1(iter2))&
                   + third*(Sy2(iter1)-Sy1(iter1))*(Sz2(iter2)-Sz1(iter2)) \&\\
             ))+curx_add_prev
             cury_adds(iter)=q*((Sy2(iter1)-Sy1(iter1))&
                   *(Sx1(iter )*Sz1(iter2)+half*(Sx2(iter )-Sx1(iter ))*Sz1(iter2)&
                   +half*Sx1(iter )*(Sz2(iter2)-Sz1(iter2))&
                   +third*(Sx2(iter )-Sx1(iter ))*(Sz2(iter2)-Sz1(iter2))&
             ))+cury_add_prevs(iter)
             curz_adds(iter,iter1)=q*((Sz2(iter2)-Sz1(iter2))&
                   *(Sx1(iter )*Sy1(iter1)+half*(Sx2(iter )-Sx1(iter ))*Sy1(iter1)&
                   +half*Sx1(iter )*(Sy2(iter1)-Sy1(iter1))&
                   +third*(Sx2(iter )-Sx1(iter ))*(Sy2(iter1)-Sy1(iter1))&
             ))+curz_add_prevs(iter,iter1)
             curx(12,1,1)=curx(12,1,1)+curx_add
             cury(12,1,1)=cury(12,1,1)+cury_adds(iter)
             curz(12,1,1)=curz(12,1,1)+curz_adds(iter,iter1)
             curx_add_prev = curx_add
          enddo
          curx_add=0.
          cury_add_prevs=cury_adds
          cury_adds=0.
       enddo
       curz_add_prevs=curz_adds
       curz adds=0.
   enddo
< #else
   ! 2d optimized
       do iter1=min(iterv1min.iterv2min).max(iterv1max.iterv2max)
          do iter=min(iterx1min.iterx2min).max(iterx1max.iterx2max)
<
             12=(i1-3+iter)+(j1-3+iter1-1)*iy
             !if(12.1t.1 .or. 12.gt.lot) then
                 print *,"index err"
print *,"lot=",lot,"12=",12
                 print *,"i1, j1",i1,j1
print *,"ix,iy",ix,iy
                 print *,"iter,iter1",iter,iter1
             !endif
             curx_add=q*((Sx2(iter)-Sx1(iter))*(Sy1(iter1)+half*(Sy2(iter1)-Sy1(iter1))))+curx_add_prev
             \verb|cury_adds(iter)=q*((Sy2(iter1)-Sy1(iter1))*(Sx1(iter))+half*(Sx2(iter)-Sx1(iter))))+cury_add_prevs(iter)|
             curz_add=-1*q*deltaz*(Sx1(iter )*Sy1(iter1)+half*(Sx2(iter)-Sx1(iter))*Sy1(iter1) &
                   + half*Sx1(iter)*(Sy2(iter1)-Sy1(iter1)) + third*(Sx2(iter)-Sx1(iter))*(Sy2(iter1)-Sy1(iter1)))
```

```
< curx(12,1,k1)=curx(12,1,k1)+curx_add
< cury(12,1,k1)=cury(12,1,k1)+cury_adds(iter)
< curz(12,1,k1)=curz(12,1,k1)+curz_add
<
 curx_add_prev=curx_add
< enddo
< curx_add=0.
< cury_add_prevs=cury_adds
< cury_adds=0.
< enddo
< #enddo
< #enddo
< #enddo
< enddo
< enddo
< cury_add_prevs=cury_adds
< cury_add_prevs=cury_adds
< cury_adds=0.
< enddo
< #endif
< in=.true.
< end subroutine densdecomp_1ord</pre>
```

5.4 densdecomp_2ord()

```
subroutine densdecomp()
< ! Charge (current) deposition on the grid, Esirkepov algorithm
< subroutine densdecomp_2ord(x2,y2,z2,x1,y1,z1,in)
   implicit none
   ! dummy variables
   logical :: in
   real(sprec), intent(in) :: x1,x2
   real(sprec), intent(in) :: y1,y2,z1,z2
   real(sprec) :: dx1,dy1,dx2,dy2,dz1,dz2,deltaz
   ! local variables
   real(sprec), DIMENSION(6)::Sx1,Sy1,Sx2,Sy2,Sz1,Sz2
   real(sprec)::curx_add,curx_add_prev,curz_add
   real(sprec), DIMENSION(6)::cury_adds,cury_add_prevs
    real(sprec), DIMENSION(6,6)::curz_adds,curz_add_prevs
    integer::i1,i2,j1,j2,k1,k2,iter,iter1,iter2, &
         iterx1min,iterx1max,itery1min,itery1max,iterz1min,iterz1max,&
         iterx2min,iterx2max,itery2min,itery2max,iterz2min,iterz2max,&
         iterxmin, iterxmax, iterymin, iterymax, iterzmin, iterzmax,&
        i,j,shifti,shiftj,shiftk,12
   i1=aint(x1)
   i2=aint(x2)
   j1=aint(y1)
   j2=aint(y2)
   k1=aint(z1)
   k2=aint(z2)
   shifti=aint(x2)-aint(x1)
   shiftj=aint(y2)-aint(y1)
   shiftk=aint(z2)-aint(z1)
   dx1=x1-aint(x1)
   dy1=y1-aint(y1)
   dx2=x2-aint(x2)
   dy2=y2-aint(y2)
   dz1=z1-aint(z1)
   dz2=z2-aint(z2)
   deltaz=z2-z1
   Sx1(:)=0.
   Sx2(:)=0.
   Sy1(:)=0.
   Sy2(:)=0.
   curx add=0.
   cury_adds=0.
   curx_add_prev=0.
   cury_add_prevs=0.
< #ifndef twoD
< Sz1(:)=0.
   Sz2(:)=0.
   curz_adds=0.
   curz_add_prevs=0.
< #else
   k1=1
   k2 = 1
   shiftk=0
   curz_add=0.
< #endif
```

```
< ! 2 order form factor
   if (dx1.le.half) then
      Sx1(2)=half*(dx1*dx1-dx1+quart)
      Sx1(4)=Sx1(2)+dx1
      Sx1(3) = one - Sx1(4) - Sx1(2)
      iterx1min=2
      iterx1max=4
   elseif (dx1.gt.half) then
      Sx1(3)=nineighth - thhalf*dx1 + half*dx1*dx1
       Sx1(5)=Sx1(3)-one+dx1
      Sx1(4) = one - Sx1(5) - Sx1(3)
      iterx1min=3
       iterx1max=5
   endif
   if (dv1.le.half) then
      Sy1(2)=half*(dy1*dy1-dy1+quart)
       Sy1(4)=Sy1(2)+dy1
      Sy1(3) = one - Sy1(4) - Sy1(2)
      itery1min=2
      itery1max=4
   elseif (dy1.gt.half) then
      Sy1(3)=nineighth - thhalf*dy1 + half*dy1*dy1
       Sy1(5)=Sy1(3)-one+dy1
      Sy1(4) = one - Sy1(5) - Sy1(3)
      itery1min=3
      itery1max=5
   endif
< #ifndef twoD</pre>
   if (dz1.le.half) then
      Sz1(2)=half*(dz1*dz1-dz1+quart)
      Sz1(4)=Sz1(2)+dz1
      Sz1(3) = one - Sz1(4) - Sz1(2)
      iterz1min=2
      iterz1max=4
   elseif (dz1.gt.half) then
      Sz1(3)=nineighth - thhalf*dz1 + half*dz1*dz1
       Sz1(5)=Sz1(3)-one+dz1
      Sz1(4) = one - Sz1(5) - Sz1(3)
      iterz1min=3
      iterz1max=5
   endif
< #endif
    if (dx2.le.half) then
       Sx2(2+shifti)=half*(dx2*dx2-dx2+quart)
       Sx2(4+shifti)=Sx2(2+shifti)+dx2
       Sx2(3+shifti)=one-Sx2(4+shifti)-Sx2(2+shifti)
      iterx2min=2+shifti
       iterx2max=4+shifti
    elseif (dx2.gt.half) then
       Sx2(3+shifti)=nineighth-thhalf*dx2+half*dx2*dx2
       Sx2(5+shifti)=Sx2(3+shifti)-one+dx2
       Sx2(4+shifti)=one-Sx2(5+shifti)-Sx2(3+shifti)
      iterx2min=3+shifti
       iterx2max=5+shifti
   endif
    if(dy2.le.half) then
      Sy2(2+shiftj)=half*(dy2*dy2-dy2+quart)
       Sy2(4+shiftj)=Sy2(2+shiftj)+dy2
       Sy2(3+shiftj)=one-Sy2(4+shiftj)-Sy2(2+shiftj)
       itery2min=2+shiftj
      itery2max=4+shiftj
    elseif(dy2.gt.half) then
       Sy2(3+shiftj)=nineighth-thhalf*dy2+half*dy2*dy2
       Sy2(5+shiftj)=Sy2(3+shiftj)-one+dy2
       Sy2(4+shiftj)=one-Sy2(5+shiftj)-Sy2(3+shiftj)
       itery2min=3+shifti
      itery2max=5+shiftj
   endif
   iterxmin=min(iterx1min,iterx2min)
   iterxmax=max(iterx1max,iterx2max)
   iterymin=min(itery1min,itery2min)
   iterymax=max(itery1max,itery2max)
< #ifndef twoD
   if(dz2.le.half) then
      Sz2(2+shiftk)=half*(dz2*dz2-dz2+quart)
       Sz2(4+shiftk)=Sz2(2+shiftk)+dz2
      Sz2(3+shiftk)=one-Sz2(4+shiftk)-Sz2(2+shiftk)
      iterz2min=2+shiftk
```

```
iterz2max=4+shiftk
    elseif(dz2.gt.half) then
       Sz2(3+shiftk)=nineighth-thhalf*dz2+half*dz2*dz2
       Sz2(5+shiftk)=Sz2(3+shiftk)-one+dz2
       Sz2(4+shiftk)=one-Sz2(5+shiftk)-Sz2(3+shiftk)
       iterz2min=3+shiftk
       iterz2max=5+shiftk
    endif
    iterzmin=min(iterz1min,iterz2min)
    iterzmax=max(iterz1max,iterz2max)
< #endif
< #ifndef twoD
    do iter2=iterzmin.iterzmax
       do iter1=iterymin,iterymax
          do iter=iterxmin.iterxmax
              12=(i1-3+iter)+(j1-3+iter1-1)*iy+(k1-3+iter2-1)*iz
              !if(12.1t.1 .or. 12.gt.lot) then
                  print *,"lot=",lot,"l2=",l2
print *,"i1, j1, k1",i1,j1,k1
                  print *,"ix,iy,iz",ix,iy,iz
<
                  print *,"iter,iter1,iter2",iter,iter1,iter2
                  print *,"index err"
             !endif
              curx_add=q*((Sx2(iter )-Sx1(iter ))&
                   *(Sy1(iter1)*Sz1(iter2)+half*(Sy2(iter1)-Sy1(iter1))*Sz1(iter2)\&
                   +half*Sy1(iter1)*(Sz2(iter2)-Sz1(iter2))&
                   +third*(Sy2(iter1)-Sy1(iter1))*(Sz2(iter2)-Sz1(iter2))&
              ))+curx_add_prev
              cury_adds(iter)=q*((Sy2(iter1)-Sy1(iter1))&
                   *(Sx1(iter )*Sz1(iter2)+half*(Sx2(iter )-Sx1(iter ))*Sz1(iter2)&
                   +half*Sx1(iter )*(Sz2(iter2)-Sz1(iter2))&
                   +third*(Sx2(iter)-Sx1(iter))*(Sz2(iter2)-Sz1(iter2))&
              ))+cury_add_prevs(iter)
              curz_adds(iter,iter1)=q*((Sz2(iter2)-Sz1(iter2))&
                   *(Sx1(iter\ )*Sy1(iter1)+half*(Sx2(iter\ )-Sx1(iter\ ))*Sy1(iter1)\&
                   +half*Sx1(iter )*(Sy2(iter1)-Sy1(iter1))&
                   +third*(Sx2(iter )-Sx1(iter ))*(Sy2(iter1)-Sy1(iter1))&
              ))+curz_add_prevs(iter,iter1)
              curx(12,1,1)=curx(12,1,1)+curx_add
              cury(12,1,1)=cury(12,1,1)+cury_adds(iter)
              curz(12,1,1)=curz(12,1,1)+curz_adds(iter,iter1)
              curx_add_prev = curx_add
          enddo
          curx_add=0.
          cury_add_prevs=cury_adds
          cury_adds=0.
       enddo
       curz_add_prevs=curz_adds
       curz_adds=0.
    enddo
< #else
       do iter1=min(itery1min,itery2min),max(itery1max,itery2max)
          do iter=min(iterx1min,iterx2min),max(iterx1max,iterx2max)
              12=(i1-3+iter)+(j1-3+iter1-1)*iy
<
              !if(12.1t.1 .or. 12.gt.lot) then
                  print *,"index err"
                  print *,"lot=",lot,"12=",12
                  print *,"i1, j1",i1,j1
<
                  print *,"ix,iy",ix,iy
print *,"iter,iter1",iter,iter1
              !endif
              curx_add=q*((Sx2(iter)-Sx1(iter))*(Sy1(iter1)+half*(Sy2(iter1)-Sy1(iter1))))+curx_add_prev
              cury_adds(iter)=q*((Sy2(iter1)-Sy1(iter1))*(Sx1(iter )+half*(Sx2(iter)-Sx1(iter))))+cury_add_prevs(iter)
curz_add=-1*q*deltaz*(Sx1(iter )*Sy1(iter1)+half*(Sx2(iter)-Sx1(iter))*Sy1(iter1) &
                   + half*Sx1(iter)*(Sy2(iter1)-Sy1(iter1)) + third*(Sx2(iter)-Sx1(iter))*(Sy2(iter1)-Sy1(iter1)))
              curx(12,1,k1)=curx(12,1,k1)+curx_add
              cury(12,1,k1)=cury(12,1,k1)+cury_adds(iter)
              curz(12,1,k1)=curz(12,1,k1)+curz_add
              curx_add_prev=curx_add
```

```
< enddo
< curx_add=0.
< cury_add_prevs=cury_adds
< cury_adds=0.
< enddo
< #endif
<
 in=.true.
< end subroutine densdecomp_2ord</pre>
```

5.5 densdecomp_3ord()

```
subroutine densdecomp()
< !
< ! Charge (current) deposition on the grid, Esirkepov algorithm
< subroutine densdecomp_3ord(x2,y2,z2,x1,y1,z1,in)</pre>
   implicit none
   ! dummy variables
   logical :: in
   real(sprec), intent(in) :: x1,x2
   real(sprec), intent(in) :: y1,y2,z1,z2
   real(sprec) :: dx1,dy1,dx2,dy2,dz1,dz2,deltaz
   ! local variables
   real(sprec), DIMENSION(6)::Sx1,Sy1,Sx2,Sy2,Sz1,Sz2
   real(sprec)::curx_add,curx_add_prev,curz_add
   real(sprec),DIMENSION(6)::cury_adds,cury_add_prevs
   real(sprec), DIMENSION(6,6)::curz_adds,curz_add_prevs
   integer::i1,i2,j1,j2,k1,k2,iter,iter1,iter2, &
         iterx1min,iterx1max,itery1min,itery1max,iterz1min,iterz1max,&
        iterx2min,iterx2max,itery2min,itery2max,iterz2min,iterz2max,&
        \texttt{iterxmin,iterxmax,iterymin,iterymax,iterzmin,iterzmax,} \&
        i,j,shifti,shiftj,shiftk,12
   i1=aint(x1)
   i2=aint(x2)
   j1=aint(y1)
   j2=aint(y2)
   k1=aint(z1)
   k2=aint(z2)
   shifti=aint(x2)-aint(x1)
   shiftj=aint(y2)-aint(y1)
   shiftk=aint(z2)-aint(z1)
   dx1=x1-aint(x1)
   dy1=y1-aint(y1)
   dx2=x2-aint(x2)
   dy2=y2-aint(y2)
   dz1=z1-aint(z1)
   dz2=z2-aint(z2)
   deltaz=z2-z1
   Sx1(:)=0.
   Sx2(:)=0.
   Sy1(:)=0.
   Sy2(:)=0.
  curx_add=0.
   cury_adds=0.
   curx_add_prev=0.
   cury_add_prevs=0.
< #ifndef twoD
< Sz1(:)=0.
   Sz2(:)=0.
   curz_adds=0.
   curz_add_prevs=0.
< #else
   k1=1
  k2=1
   shiftk=0
   curz_add=0.
< #endif
< 1-----
< ! 3 order form factor
< 1-----
     if (dx1.le.half) then
         Sx1(2) = negsixth*(dx1-one)*(dx1-one)*(dx1-one) !6
```

```
Sx1(3) = twoth+half*(dx1-two)*dx1*dx1 !5
                Sx1(5) = sixth *dx1*dx1*dx1 !3
               Sx1(4) = one-Sx1(5)-Sx1(3)-Sx1(2)!sixth*(one+three*dx1*(one+dx1-dx1*dx1)) !7
               iterx1min = 2
               iterx1max = 5
        elseif (dx1.gt.half) then
              Sx1(5) = sixth*dx1*dx1*dx1 !3
               Sx1(4)=twoth+half*(negone-dx1)*(one-dx1)*(one-dx1) !7
               Sx1(2)=sixth*(one-dx1)*(one-dx1)*(one-dx1) !6
               Sx1(3) = one - Sx1(5) - Sx1(4) - Sx1(2) ! Sx1(3) = sixth*(one+three*(one-dx1)*(two-(one-dx1)*(one-dx1)-dx1)) !10
               iterx1min = 2
               iterx1max = 5
          endif
          if (dv1.le.half) then
                Sy1(2) = negsixth*(dy1-one)*(dy1-one)*(dy1-one) !6
               Sy1(3) = twoth + half*(dy1-two)*dy1*dy1 !5
               Sv1(5) = sixth *dv1*dv1*dv1 !3
               Sy1(4) = one-Sy1(5)-Sy1(3)-Sy1(2)!sixth*(one+three*dy1*(one+dy1-dy1*dy1)) !7
<
               itery1min = 2
               itery1max = 5
<
        elseif (dy1.gt.half) then
               Sv1(5) = sixth*dv1*dv1*dv1 !3
               Sy1(4)=twoth+half*(negone-dy1)*(one-dy1)*(one-dy1) !7
               Sy1(2)=sixth*(one-dy1)*(one-dy1)*(one-dy1)!6
               <
               itery1min = 2
                itery1max = 5
          endif
< #ifndef twoD
          if (dz1.le.half) then
               Sz1(2) = negsixth*(dz1-one)*(dz1-one)*(dz1-one) !6
               Sz1(3) = twoth + half*(dz1-two)*dz1*dz1 !5
               Sz1(5) = sixth *dz1*dz1*dz1 !3
               Sz1(4) = one-Sz1(5)-Sz1(3)-Sz1(2)!sixth*(one+three*dz1*(one+dz1-dz1*dz1)) !7
<
                iterz1min = 2
               iterz1max = 5
        elseif (dz1.gt.half) then
               Sz1(5)=sixth*dz1*dz1*dz1!3
                {\tt Sz1(4)=twoth+half*(negone-dz1)*(one-dz1)*(one-dz1)} \end{\ensuremath{\mbox{!}}} ?
               Sz1(2)=sixth*(one-dz1)*(one-dz1)*(one-dz1) !6
               iterz1min = 2
                iterz1max = 5
           endif
< #endif
          if (dx2.le.half) then
                Sx2(2+shifti) = negsixth*(dx2-one)*(dx2-one)*(dx2-one) !6
                Sx2(3+shifti) = twoth+half*(dx2-two)*dx2*dx2 !5
                Sx2(5+shifti) = sixth *dx2*dx2*dx2 !3
               iterx2min = 2+shifti
               iterx2max = 5+shifti
        elseif (dx2.gt.half) then
             Sx2(5+shifti)=sixth*dx2*dx2*dx2!3
               Sx2(4+shifti)=twoth+half*(negone-dx2)*(one-dx2)*(one-dx2) !7
               Sx2(2+shifti)=sixth*(one-dx2)*(one-dx2)*(one-dx2) !6
               Sx2(3+shifti)=one-Sx2(5+shifti)-Sx2(4+shifti)-Sx2(2+shifti)
               iterx2min = 2+shifti
               iterx2max = 5+shifti
          endif
          if (dy2.le.half) then
               Sy2(2+shiftj) = negsixth*(dy2-one)*(dy2-one)*(dy2-one) !6
               Sy2(3+shiftj)= twoth+half*(dy2-two)*dy2*dy2 !5
               Sy2(5+shiftj) = sixth *dy2*dy2*dy2 !3
               Sy2(4+shiftj)= one-Sy2(5+shiftj)-Sy2(3+shiftj)-Sy2(2+shiftj)
               itery2min = 2+shiftj
               itery2max = 5+shiftj
         elseif (dv2.gt.half) then
               Sv2(5+shifti)=sixth*dv2*dv2*dv2!3
               {\tt Sy2(4+shiftj)=twoth+half*(negone-dy2)*(one-dy2)*(one-dy2)} \end{subarray} \e
               Sy2(2+shiftj)=sixth*(one-dy2)*(one-dy2)*(one-dy2)!6
               Sy2(3+shiftj)=one-Sy2(5+shiftj)-Sy2(4+shiftj)-Sy2(2+shiftj)
               itery2min = 2+shiftj
itery2max = 5+shiftj
<
          endif
          iterxmin=min(iterx1min,iterx2min)
          iterxmax=max(iterx1max,iterx2max)
          iterymin=min(itery1min,itery2min)
          iterymax=max(itery1max,itery2max)
< #ifndef twoD
<
          if (dz2.le.half) then
                Sz2(2+shiftk) = negsixth*(dz2-one)*(dz2-one)*(dz2-one) !6
                Sz2(3+shiftk) = twoth+half*(dz2-two)*dz2*dz2 !5
```

```
Sz2(5+shiftk) = sixth *dz2*dz2*dz2 !3
          Sz2(4+shiftk)= one-Sz2(5+shiftk)-Sz2(3+shiftk)-Sz2(2+shiftk)
          iterz2min = 2+shiftk
          iterz2max = 5+shiftk
     elseif (dz2.gt.half) then
          Sz2(5+shiftk)=sixth*dz2*dz2*dz2!3
         Sz2(4+shiftk)=twoth+half*(negone-dz2)*(one-dz2)*(one-dz2) !7
         Sz2(2+shiftk)=sixth*(one-dz2)*(one-dz2)*(one-dz2)!6
         Sz2(3+shiftk)=one-Sz2(5+shiftk)-Sz2(4+shiftk)-Sz2(2+shiftk)
         iterz2min = 2+shiftk
         iterz2max = 5+shiftk
       endif
       iterzmin=min(iterz1min,iterz2min)
      iterzmax=max(iterz1max,iterz2max)
< #endif
< #ifndef twoD
   do iter2=iterzmin.iterzmax
      do iter1=iterymin,iterymax
         do iter=iterxmin,iterxmax
             12=(i1-3+iter)+(j1-3+iter1-1)*iy+(k1-3+iter2-1)*iz
             curx_add=q*((Sx2(iter )-Sx1(iter ))&
     *(Sy1(iter1)*Sz1(iter2)+half*(Sy2(iter1)-Sy1(iter1))*Sz1(iter2)&
                  +half*Sy1(iter1)*(Sz2(iter2)-Sz1(iter2))&
                  + third*(Sy2(iter1)-Sy1(iter1))*(Sz2(iter2)-Sz1(iter2)) \&\\
             ))+curx_add_prev
             cury_adds(iter)=q*((Sy2(iter1)-Sy1(iter1))&
                  *(Sx1(iter )*Sz1(iter2)+half*(Sx2(iter )-Sx1(iter ))*Sz1(iter2)&
                  +half*Sx1(iter )*(Sz2(iter2)-Sz1(iter2))&
                  +third*(Sx2(iter )-Sx1(iter ))*(Sz2(iter2)-Sz1(iter2))&
             ))+cury_add_prevs(iter)
             curz_adds(iter,iter1)=q*((Sz2(iter2)-Sz1(iter2))&
                  *(Sx1(iter )*Sy1(iter1)+half*(Sx2(iter )-Sx1(iter ))*Sy1(iter1)&
                  +half*Sx1(iter )*(Sy2(iter1)-Sy1(iter1))&
                  +third*(Sx2(iter )-Sx1(iter ))*(Sy2(iter1)-Sy1(iter1))&
             ))+curz_add_prevs(iter,iter1)
             curx(12,1,1)=curx(12,1,1)+curx_add
             cury(12,1,1) = cury(12,1,1) + cury_adds(iter)
             curz(12,1,1)=curz(12,1,1)+curz_adds(iter,iter1)
            curx_add_prev = curx_add
         enddo
         curx_add=0.
         cury_add_prevs=cury_adds
          cury_adds=0.
      enddo
      curz_add_prevs=curz_adds
      curz_adds=0.
   enddo
< #else
   ! 2d optimized
       do iter1=min(itery1min,itery2min),max(itery1max,itery2max)
         do iter=min(iterx1min,iterx2min),max(iterx1max,iterx2max)
            12=(i1-3+iter)+(j1-3+iter1-1)*iy
             curx_add=q*((Sx2(iter)-Sx1(iter))*(Sy1(iter1)+half*(Sy2(iter1)-Sy1(iter1))))+curx_add_prev
             cury_adds(iter)=q*((Sy2(iter1)-Sy1(iter1))*(Sx1(iter )+half*(Sx2(iter)-Sx1(iter))))+cury_add_prevs(iter)
             curz_add=-1*q*deltaz*(Sx1(iter )*Sy1(iter1)+half*(Sx2(iter)-Sx1(iter))*Sy1(iter1) &
                  +half*Sx1(iter)*(Sy2(iter1)-Sy1(iter1))+third*(Sx2(iter)-Sx1(iter))*(Sy2(iter1)-Sy1(iter1)))
             curx(12,1,k1)=curx(12,1,k1)+curx add
             cury(12,1,k1)=cury(12,1,k1)+cury_adds(iter)
             curz(12,1,k1)=curz(12,1,k1)+curz_add
            curx_add_prev=curx_add
          enddo
          curx_add=0.
          cury_add_prevs=cury_adds
          cury_adds=0.
       enddo
< #endif
       in=.true.
< end subroutine densdecomp_3ord
```

5.6 inject_others()

1370c726

```
perz = sign(.5*(mz-1.*nghostz), p(ions) \%z-1.*(nghostz/2+1)) + sign(.5*(mz-1.*nghostz), p(ions) \%z-mz + 1.*(nghostz/2+1)) + sign(.5*(mz-1.*nghostz), p(ions) \%z-mz + 1.*(nghostz), p(ions) \%z-mz +
                                               perz=sign(.5*(mz-5.),p(ions)%z-3.)+sign(.5*(mz-5.),p(ions)%z-mz+2.)
1380c736
                                                                       perz=-(mzl(k1+1)-1.*nghostz)
                                                                      perz=-(mzl(k1+1)-5.)
1426c782
                       perz=sign(.5*(mz-1.*nghostz),p(ions)%z-1.*(nghostz/2+1))+sign(.5*(mz-1.*nghostz),p(ions)%z-mz +1.*(nghostz/2))
<
                       perz=sign(.5*(mz-5.),p(ions)%z-3.)+sign(.5*(mz-5.),p(ions)%z-mz +2.)
1435c791
                                                                       perz=-(mzl(k1+1)-1.*nghostz)
<
                                                                       perz=-(mzl(k1+1)-5.)
1482c838
                       \verb"perz=sign" (.5*(mz-1.*nghostz)", p(maxhlf+lecs) \% z-1.*(nghostz/2+1)) \&
<
                                                                         + sign(.5*(mz-1.*nghostz), p(maxhlf+lecs)\%z-mz +1.*(nghostz/2))\\
<
                       perz = sign(.5*(mz-5.), p(maxhlf+lecs)\%z-3.) + sign(.5*(mz-5.), p(maxhlf+lecs)\%z-mz + 2.)
1489c845
                                                                      perz=-(mzl(k1+1)-1.*nghostz)
                                                                       perz=-(mzl(k1+1)-5.)
1538c894
                       \verb"perz=sign" (.5*(mz-1.*nghostz)", p(maxhlf+lecs) %z-1.*(nghostz/2+1)) & \\
<
<
                                                                       +sign(.5*(mz-1.*nghostz),p(maxhlf+lecs)%z-mz+1.*(nghostz/2))
---
                       perz = sign(.5*(mz-5.), p(maxhlf+lecs)\%z-3.) + sign(.5*(mz-5.), p(maxhlf+lecs)\%z-mz +2.)
1545c901
                                                                       perz=-(mzl(k1+1)-1.*nghostz)
___
                                                                       perz=-(mzl(k1+1)-5.)
1596c952
                                               pery=sign(.5*(my-1.*nghost),p(ions)%y-1.*(nghost/2+1))+sign(.5*(my-1.*nghost),p(ions)%y-my+1.*(nghost/2))
---
                                               pery=sign(.5*(my-5.),p(ions)%y-3.)+sign(.5*(my-5.),p(ions)%y-my+2.)
1601c957
                                                                       pery=-(myl(j1+1)-1.*nghost)
___
                                                                       pery=-(myl(j1+1)-5.)
1641c997
                                               pery = sign(.5*(my-1.*nghost), p(ions)\%y-1.*(nghost/2+1)) + sign(.5*(my-1.*nghost), p(ions)\%y-my+1.*(nghost/2)) + sign(.5*(my-1.*nghost), p(ions)\%y-my+1.*(nghost/2+1)) + sign(.5*(my-1.*nghost), p(ions)\%y-my+1.*(nghost), 
---
                                               pery=sign(.5*(my-5.),p(ions)%y-3.)+sign(.5*(my-5.),p(ions)%y-my+2.)
1646c1002
                                                                       pery=-(myl(j1+1)-1.*nghost)
                                                                       pery=-(myl(j1+1)-5.)
1687c1043
                                               pery=sign(.5*(my-1.*nghost),p(maxhlf+lecs)%y-1.*(nghost/2+1))&
                                                                    +sign(.5*(my-1.*nghost),p(maxhlf+lecs)%y-my+1.*(nghost/2))
                                               pery = sign(.5*(my-5.), p(maxhlf+lecs)\%y-3.) + sign(.5*(my-5.), p(maxhlf+lecs)\%y-my+2.)
1692c1048
                                                                       pery=-(myl(j1+1)-1.*nghost)
                                                                      pery=-(myl(j1+1)-5.)
1733c1089
                                               pery=sign(.5*(my-1.*nghost),p(maxhlf+lecs)%y-1.*(nghost/2+1))&
<
                                                                    +sign(.5*(my-1.*nghost),p(maxhlf+lecs)%y-my+1.*(nghost/2))
                                               pery = sign(.5*(my-5.), p(maxhlf+lecs)\%y-3.) + sign(.5*(my-5.), p(maxhlf+lecs)\%y-my+2.)
1738c1094
                                                                      pery=-(myl(j1+1)-1.*nghost)
<
                                                                       pery=-(myl(j1+1)-5.)
```

5.7 init_maxw_table()

This next change is unrelated to current deposit, but is a small improvement to the PDF used for initialization of the particles. The arrays pdf_table_e and pdf_table_i are set to be of dimension pdf_sz+1, then elements from 2 to pdf_sz+1 are computed as the prefix sum of func. Without this change, pdf_table_e and pdf_table_i are not large enough to contain all elements in the cumulative sum of func, so one element is skipped over (i.e., sum(func(1:1))). This leads to a sharp feature between bins 1 and 2 of the PDFs, but is removed via the modification below.

5.8 inject_plasma_region()

```
2495,2496c1853
        real, dimension(pdf_sz) :: gamma_table_i, gamma_table_e
          real, dimension(pdf_sz+1) :: pdf_table_i, pdf_table_e
        real, dimension(pdf_sz) :: pdf_table_i, gamma_table_i, pdf_table_e, gamma_table_e
2549,2550c1906,1907
       iglob_min=(nghost/2+1)+mxcum
<
        iglob_max=(mx-(nghost/2))+mxcum
        iglob_min=3+mxcum
        iglob_max=(mx-2)+mxcum
2552,2553c1909,1910
       minx=1.*(nghost/2+1)
        maxx=1.*(nghost/2+1)
2563,2566c1920,1923
       if(inject_minx<iglob_min) minx=1.*(nghost/2+1)</pre>
        if(inject_maxx<iglob_min) maxx=1.*(nghost/2+1)</pre>
        if(inject_minx>=iglob_max) minx=mx-(nghost/2)
        if(inject_maxx>=iglob_max) maxx=mx-(nghost/2)
        if(inject_minx<iglob_min) minx=3.</pre>
        if(inject_maxx<iglob_min) maxx=3.</pre>
        if(inject_minx>=iglob_max) minx=mx-2
        if(inject_maxx>=iglob_max) maxx=mx-2
2577,2578c1934,1935
        jglob_min=(nghost/2+1)+mycum !global extent of the y boundaries on this processor
        jglob_max=(my-(nghost/2))+mycum
        jglob_min=3+mycum !global extent of the y boundaries on this processor
        jglob_max=(my-2)+mycum
2580,2581c1937,1938
       minv=1.*(nghost/2+1)
       maxy=1.*(nghost/2+1)
       miny=3.
       maxy=3.
2595,2598c1952,1955
       if(inject_miny<jglob_min) miny=1.*(nghost/2+1)</pre>
        if(inject_maxy<jglob_min) maxy=1.*(nghost/2+1)</pre>
        if(inject_miny>=jglob_max) miny=my-nghost/2
        if(inject_maxy>=jglob_max) maxy=my-nghost/2
<
        if(inject_miny<jglob_min) miny=3.</pre>
        if(inject_maxy<jglob_min) maxy=3.</pre>
        if(inject_miny>=jglob_max) miny=my-2
        if(inject_maxy>=jglob_max) maxy=my-2
2619,2620c1976,1977
       maxz=1.*(nghostz/2+1)+1.
<
       minz=1.*(nghostz/2+1)
       maxz=4.
       minz=3.
2626,2627c1983,1984
        kglob_min=(nghostz/2+1)+mzcum !global extent of the y boundaries on this processor
        kglob_max=(mz-(nghostz/2))+mzcum
---
        kglob_min=3+mzcum !global extent of the y boundaries on this processor
2629,2630c1986,1987
       minz=1.*(nghostz/2+1)
       maxz=1.*(nghostz/2+1)
2640,2643c1997,2000
        if(inject_minz<kglob_min) minz=1.*(nghostz/2+1)</pre>
        if(inject_maxz<kglob_min) maxz=1.*(nghostz/2+1)</pre>
        if(inject_minz>=kglob_max) minz=mz-1.*(nghostz/2)
        if(inject_maxz>=kglob_max) maxz=mz-1.*(nghostz/2)
        if(inject_minz<kglob_min) minz=3.</pre>
        if(inject_maxz<kglob_min) maxz=3.</pre>
        if(inject_minz>=kglob_max) minz=mz-2.
        if(inject_maxz>=kglob_max) maxz=mz-2.
2737,2739c2089,2091
                         values(1)=(p(ions)%x-1.*(nghost/2+1))/c_omp
                         values(2)=((p(ions)%y+modulo(rank,sizey)*(myall-nghost)) -1.*(nghost/2+1))/c_omp
                         values(3)=((p(ions)%z+(rank/sizey)*(mzall-nghostz))-1.*(nghostz/2+1))/c_omp
                         values(1)=(p(ions)%x-3.)/c omp
```

6 particles_movedeposit.F90

6.1 particles_movedeposit()

A mover routine, consistent with the current deposit, is called (mover for zigzag, mover_lord for 1st order density decomposition, mover_2ord for 2^{nd} order, mover_3ord for 3^{rd}). The routines mover_lord, mover_2ord, and mover_3ord differ only by shape function definition. For the density decomposition mover routines, fields are computed as the sum of the particle shape function multiplied by the field at (primal) gridpoints. In 3D, the fields at gridpoints are computed via linear interpolation of the fields defined on the Yee lattice. These interpolated arrays are denoted by ex_p, ey_p, ez_p, bx_p, by_p, bz_p. The 2D case is a similar operation, but uses shifted particle shape functions (to align with gridpoints on the Yee lattice) and fields defined on the Yee lattice. This difference between 2D and 3D implementations (i.e. for the 2D implementation, the use of particle shape functions defined at Yee lattice points in conjunction with the EM fields defined on the Yee lattice, and in 3D the use of shape functions defined at primal gridpoints in conjunction with EM fields defined at primal gridpoints) is not chosen for any fundamental reason, it is just the state they were left in after optimization of the 2D and 3D mover routines. The 2D mover routine could be changed to match the 3D version.

```
69,85c69,71
< #ifdef zzag
                      call mover(1,ions,qmi)
                      call mover(1+maxhlf,lecs+maxhlf,qme) ! electrons
< #endif
< #ifdef dd1
                      call mover_1ord(1,ions,qmi)
                      call mover_1ord(1+maxhlf,lecs+maxhlf,qme) ! electrons
< #endif
< #ifdef dd2
                      call mover_2ord(1,ions,qmi)
                                                                   ! ions
                      call mover_2ord(1+maxhlf,lecs+maxhlf,qme) ! electrons
< #endif
< #ifdef dd3
                      call mover_3ord(1,ions,qmi)
                                                                   ! ions
                      call mover_3ord(1+maxhlf,lecs+maxhlf,qme) ! electrons
< #endif
               call mover(1,ions,qmi)
               call mover(1+maxhlf,lecs+maxhlf,qme) ! electrons
```

6.2 mover 1ord()

```
350,1274d340
                                                 subroutine mover 1ord()
<!
<!
< subroutine mover_1ord(n1,n2,qm)
       implicit none
       ! dummy variables
       integer, intent(in) :: n2, n1
       real(sprec), intent(in) :: qm
       ! local variables
         integer :: iter1,iter2,iter3,iter1min,iter1max,iter2min,iter2max,iter3min,iter3max
         real, DIMENSION(6) :: Sxp,Syp,Sxd,Syd,Szp,Szd
       integer :: npr,l,n,ip,jp,kp,id,jd,kd
          integer :: lpp,lpd, ldp, ldd
         integer :: lppp
        real dxp, dyp, dzp, dxd, dyd, dzd, f, g, ex0, ey0, ez0, bx0, by0, bz0
```

```
real u0,v0,w0,u1,v1,w1, cinv, g1, corrqm
                 real qm0
                     logical :: cond1, cond2, cond3, cond4
<!, xglob, yglob, gammawall, betawall, gamma, walloc
<! real vdriftx, vdrifty, gdrift, decrem</pre>
                 integer ::yes_gammacut
                 real gammacut
< #ifdef vay
                 real ustar, sig, tx, ty, tz, vx0, vy0, vz0
                       real bx_ext, by_ext, bz_ext, ex_ext, ey_ext, ez_ext
                      real chival, threed
                       real exsc, eysc, ezsc, bxsc, bysc, bzsc, v3x0, v3y0, v3z0
                      real up, vp, wp, gampinv, ppinv, gamp, dragx, dragy, dragz, lfx, lfy, lfz, edotv, lsq
<
                       \verb|real| bx00, by00, bz00, drag coeff, drag thresh, \verb|reductionfactor||
                       integer redLL
                      real gammathinv
<
<
                      \verb"real,dimension(mx,my,mz)::= x_p, ey_p, ez_p, bx_p, by_p, bz_p"
                      ! primal grids
                       ex_p=0.5*(ex+cshift(ex,-1,dim=1))
                       ey_p=0.5*(ey+cshift(ey,-1,dim=2))
                       ez_p=0.5*(ez+cshift(ez,-1,dim=3))
                      bx_p=0.5*(bx+cshift(bx,-1,dim=2))
                       by_p=0.5*(by+cshift(by,-1,dim=1))
                       bz_p=0.5*(0.5*(bz+cshift(bz,-1,dim=1))&
                                  +0.5*(\texttt{cshift(bz,-1,dim=2)}+\texttt{cshift(cshift(bz,-1,dim=2),-1,dim=1))})
< !user stripe cooling
< redLL=1 ! if 1 then use reduced Landau Lifshits, otherwise Hededal (apart from 1/beta^2)
\mbox{\ensuremath{$<$}}\mbox{\ensuremath{$d$}}\mbox{\ensuremath{$d$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a$}}\mbox{\ensuremath{$a
       gammathinv=1./(1.+3.*delgam)
< !end user stripe cooling
< 1
                  real pcosth, pphi, psinth, v0t, ut1, vt1, wt1, gam
< !
                 real ptx, pty, ptz
<
                 cinv=1./c
                  qm0=qm
                 do n=n1,n2
                                     ip=aint(p(npr)%x)
                                     dxp=p(npr)%x-ip
                                     jp=aint(p(npr)%y)
                                     dyp=p(npr)%y-jp
                                     kp=aint(p(npr)%z)
                                         Sxp(:)=0.
                                         Syp(:)=0.
                                        id=aint(p(npr)%x-half)
                                     dxd=p(npr)%x-half-id
                                     jd=aint(p(npr)%y-half)
                                     dyd=p(npr)%y-half-jd
                                     kd=aint(p(npr)%z-half)
                                         Sxd(:)=0.
                                         Syd(:)=0.
< #ifndef twoD</pre>
                                         dzp=p(npr)%z-kp
                                         Szp(:)=0.
                                         dzd=(p(npr)%z-half)-kd
                                         Szd(:)=0.
< #endif
        !O order form factor Sxp(3)=1.-dxp
         Sxp(4)=dxp
         Sxd(3)=1.-dxd
         Sxd(4)=dxd
        iter1min=3
        iter1max=4
         Syp(3)=1.-dyp
         Syp(4)=dyp
         Syd(3)=1.-dyd
         Syd(4)=dyd
         iter2min=3
         iter2max=4
```

```
< #ifndef twoD
   Szp(3)=1.-dzp
    Szp(4)=dzp
   Szd(3)=1.-dzd
   Szd(4)=dzd
   iter3min=3
   iter3max=4
< #endif
   ex0=0.
   ey0=0.
   ez0=0.
   bx0=0.
   bv0=0.
   bz0=0.
< #ifndef twoD
   do iter3=iter3min.iter3max
       do iter2=iter2min,iter2max
             ! lppp = (ip-3+iter1)+iy*(jp-3+iter2-1)+iz*(kp-3+iter3-1)
             ! \verb| if (lppp.ge.1 .and. lppp.le.lot)| then
                  print *, "out of range"
             !endif
                \verb|ex0=ex0+sum(ex_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)|
                \verb| ey0=ey0+sum(ey_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)|
                 \tt ez0=ez0+sum(ez\_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3) 
                \texttt{bx0-bx0+sum(bx\_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)}
                \verb|by0=by0+sum(by_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)|
                \texttt{bz0-bz0+sum(bz-p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)}
       enddo
   enddo
< #else
    do iter2=iter2min,iter2max
       do iter1=iter1min,iter1max
          lpp=(ip-3+iter1)+iy*(jp-3+iter2-1)
          lpd=(ip-3+iter1)+iy*(jd-3+iter2-1)
<
          ldp=(id-3+iter1)+iy*(jp-3+iter2-1)
          ldd=(id-3+iter1)+iy*(jd-3+iter2-1)
          ex0=ex0+ex(ldp,1,1)*Sxd(iter1)*Syp(iter2)
          ey0=ey0+ey(lpd,1,1)*Sxp(iter1)*Syd(iter2)
          ez0=ez0+ez(lpp,1,1)*Sxp(iter1)*Syp(iter2)
          bx0=bx0+bx(lpd,1,1)*Sxp(iter1)*Syd(iter2)
          by0=by0+by(ldp,1,1)*Sxd(iter1)*Syp(iter2)
          bz0=bz0+bz(ldd,1,1)*Sxd(iter1)*Syd(iter2)
       enddo
    \verb"enddo"
< #endif
    ex0=0.5*ex0*qm
   ey0=0.5*ey0*qm
    ez0=0.5*ez0*qm
   bx0=0.5*bx0*qm*cinv
   by0=0.5*by0*qm*cinv
   bz0=0.5*bz0*qm*cinv
   if(external_fields) then
       call get_external_fields(real(p(npr)%x,sprec),p(npr)%y,&
            p(npr)%z,ex_ext,ey_ext,ez_ext,bx_ext,by_ext,bz_ext)
       bx0=bx0+bx_ext*0.5*qm*cinv
       by0=by0+by_ext*0.5*qm*cinv
       bz0=bz0+bz_ext*0.5*qm*cinv
      ex0=ex0+ex ext*0.5*qm
      ey0=ey0+ey_ext*0.5*qm
      ez0=ez0+ez_ext*0.5*qm
    !to be used later for synchrotron
   bx00=bx0
   bv00=bv0
   bz00=bz0
<
       First half electric acceleration, with relativity's gamma:
< #ifdef vay
   !Use Vay 2008 particle mover
    g=1./sqrt(1.+p(npr)\%u**2+p(npr)\%v**2+p(npr)\%w**2) \ !reciprocal \ of \ the \ Lorentz \ factor
    vx0=c*p(npr)%u*g !3-velocity of the particle
   vy0=c*p(npr)%v*g
   vz0=c*p(npr)%w*g
   u1=c*p(npr)%u+2.*ex0+vy0*bz0-vz0*by0 !uprime, taking into account
```

```
!that cinv is already incorporated within B
   v1=c*p(npr)%v+2.*ey0+vz0*bx0-vx0*bz0
   w1=c*p(npr)%w+2.*ez0+vx0*by0-vy0*bx0
   !Lorentz factor for uprime
   ustar=cinv*(u1*bx0+v1*by0+w1*bz0)
   sig=cinv*cinv*(c**2+u1**2+v1**2+w1**2)-(bx0**2+by0**2+bz0**2)
   g=1./sqrt(0.5*(sig+sqrt(sig**2+4.*(bx0**2+by0**2+bz0**2+ustar**2))))
   tx=bx0*g
   ty=by0*g
   tz=bz0*g
f=1./(1.+tx**2+ty**2+tz**2)
   u0=f*(u1+(u1*tx+v1*ty+w1*tz)*tx+v1*tz-w1*ty)
   v0=f*(v1+(u1*tx+v1*ty+w1*tz)*ty+w1*tx-u1*tz)
   w0=f*(w1+(u1*tx+v1*ty+w1*tz)*tz+u1*ty-v1*tx)
< #else
  !Use Boris algorithm
<
      First half electric acceleration, with Lorentz gamma:
   u0=c*p(npr)%u+ex0
   v0=c*p(npr)%v+ey0
   w0=c*p(npr)%w+ez0
   ! First half magnetic rotation, with Lorentz gamma: g=c/sqrt(c**2+u0**2+v0**2+v0**2)
<
   bx0=g*bx0
   by0=g*by0
   bz0=g*bz0
   f=2./(1.+bx0*bx0+by0*by0+bz0*bz0)
   u1=(u0+v0*bz0-w0*by0)*f
   v1 = (v0 + w0 * bx0 - u0 * bz0) * f
   w1 = (w0 + u0 * by0 - v0 * bx0) * f
   ! Second half mag. rot'n & el. acc'n:
   u0=u0+v1*bz0-w1*by0+ex0
   v0=v0+w1*bx0-u1*bz0+ey0
   w0=w0+u1*by0-v1*bx0+ez0
< #endif
    !user stripe
    !following tamburrini, cooling is implemented at this point,
   !after the Lorentz push
      Get normalized 4-velocity:
   p(npr)%u=u0*cinv
   p(npr)%v=v0*cinv
   p(npr)%w=w0*cinv
   ! freeze particles, to verify the generation of the correct fields
   ! (the three lines above should also be commented out)
                        p(npr)%u=p(npr)%u
                         p(npr)%v=p(npr)%v
                         p(npr)%w=p(npr)%w
   ! end stripe user
      Position advance:
   g=c/sqrt(c**2+u0**2+v0**2+w0**2)
   p(npr)%x=p(npr)%x + p(npr)%u*g*c
   p(npr)%y=p(npr)%y + p(npr)%v*g*c
   p(npr)%z=p(npr)%z + p(npr)%w*g*c
< enddo
< end subroutine mover_1ord
6.3 mover_2ord()
                                              subroutine mover 2ord()
<!
<!
     _____
< subroutine mover_2ord(n1,n2,qm)
       implicit none
       ! dummy variables
       integer, intent(in) :: n2, n1
       real(sprec), intent(in) :: qm
```

! local variables

```
integer :: iter1,iter2,iter3,iter1min,iter1max,iter2min,iter2max,iter3min,iter3max
         real, DIMENSION(6) :: Sxp,Syp,Sxd,Syd,Szp,Szd
        integer :: npr,l,n,ip,jp,kp,id,jd,kd
         integer :: lpp,lpd, ldp, ldd
          integer :: lppp
       real dxp,dyp,dzp,dxd,dyd,dzd,f,g,ex0,ey0,ez0,bx0,by0,bz0
       real u0,v0,w0,u1,v1,w1, cinv, g1, corrqm
<
       real am0
         logical :: cond1, cond2, cond3, cond4
< !, xglob, yglob, gammawall, betawall, gamma, walloc
       real vdriftx, vdrifty, gdrift, decrem
<
< !
       integer ::yes_gammacut
< !
       real gammacut
< #ifdef vay
<
       real ustar, sig, tx, ty, tz, vx0, vy0, vz0
< #endif
          \verb"real" bx_ext", by_ext", bz_ext", ex_ext", ey_ext", ez_ext"
          real chival, threed
<
          real exsc, eysc, ezsc, bxsc, bysc, bzsc, v3x0, v3y0, v3z0
          real up,vp,wp,gampinv,ppinv,gamp,dragx,dragy,dragz,lfx,lfy,lfz,edotv,lsq
          real bx00, by00, bz00, dragcoeff, dragthresh, reduction factor
<
          integer redLL
         real gammathinv
<
         real, dimension(mx, my, mz)::ex_p, ey_p, ez_p, bx_p, by_p, bz_p
          ! primal grids
          ex_p=0.5*(ex+cshift(ex,-1,dim=1))
          ey_p=0.5*(ey+cshift(ey,-1,dim=2))
          ez_p=0.5*(ez+cshift(ez,-1,dim=3))
          bx_p=0.5*(bx+cshift(bx,-1,dim=2))
          by_p=0.5*(by+cshift(by,-1,dim=1))
          bz_p=0.5*(0.5*(bz+cshift(bz,-1,dim=1))&
               +0.5*(\texttt{cshift(bz,-1,dim=2)}+\texttt{cshift(cshift(bz,-1,dim=2),-1,dim=1))})
          !bz_p=0.5*(bz_p + cshift(bz_p,-1,dim=3))
< !user stripe cooling
< redLL=1 ! if 1 then use reduced Landau Lifshits, otherwise Hededal (apart from 1/beta^2)
< dragthresh=1e-1 ! maximum differential change in momentum
< gammathinv=1./(1.+3.*delgam)
< !end user stripe cooling
        real pcosth, pphi, psinth, v0t, ut1, vt1, wt1, gam
< !
       real ptx, pty, ptz
       cinv=1./c
       qm0=qm
       do n=n1,n2
                npr=n
                ip=aint(p(npr)%x)
                dxp=p(npr)%x-ip
                jp=aint(p(npr)%y)
                dyp=p(npr)%y-jp
                kp=aint(p(npr)%z)
                  Sxp(:)=0.
                  Syp(:)=0.
                  id=aint(p(npr)%x-half)
<
                dxd=p(npr)%x-half-id
                jd=aint(p(npr)%y-half)
                dyd=p(npr)%y-half-jd
                kd=aint(p(npr)%z-half)
                  Sxd(:)=0.
                  Syd(:)=0.
< #ifndef twoD
                  dzp=p(npr)%z-kp
                  Szp(:)=0.
                  dzd=(p(npr)%z-half)-kd
                  Szd(:)=0.
< #endif
                  if (dxp.le.half) then
                     Sxp(2) = half * (dxp*dxp-dxp+quart)
                     Sxp(4) = Sxp(2) + dxp
<
                     Sxp(3) = one-Sxp(4)-Sxp(2)
                     iter1min=2
```

```
iter1max=4
                    elseif(dxp.gt.half) then
                        Sxp(3) = nineighth - thhalf*dxp + half*dxp*dxp
                        Sxp(5) = Sxp(3) - one + dxp
                        Sxp(4) = one-Sxp(5)-Sxp(3)
                        iter1min=3
                        iter1max=5
                    endif
                    if (dyp.le.half) then
                        Syp(2) = half * (dyp*dyp-dyp+quart)
                        Syp(4) = Syp(2) + dyp
                        Syp(3) = one-Syp(4)-Syp(2)
                        iter2min=2
                        iter2max=4
                    elseif(dyp.gt.half) then
                       Syp(3) = nineighth - thhalf*dyp + half*dyp*dyp
Syp(5) = Syp(3)-one+dyp
                        Syp(4) = one-Syp(5)-Syp(3)
                        iter2min=3
                       iter2max=5
                    endif
< #ifndef twoD
                    \quad \text{if } \text{(dzp.le.half) then} \\
                       Szp(2) = half * (dzp*dzp-dzp+quart)

Szp(4) = Szp(2)+dzp
                        Szp(3) = one-Szp(4)-Szp(2)
<
                        iter3min=2
                        iter3max=4
                    elseif(dzp.gt.half) then
                       Szp(3) = nineighth - thhalf*dzp + half*dzp*dzp
Szp(5) = Szp(3)-one+dzp
                        Szp(4) = one-Szp(5)-Szp(3)
                        iter3min=3
                        iter3max=5
                    endif
< #endif
                    if (dxd.le.half) then
                       Sxd(2) = half * (dxd*dxd-dxd+quart)
Sxd(4) = Sxd(2)+dxd
                        Sxd(3) = one-Sxd(4)-Sxd(2)
                        iter1min=2
                        iter1max=4
                    elseif(dxd.gt.half) then
                       Sxd(3) = nineighth - thhalf*dxd + half*dxd*dxd
Sxd(5) = Sxd(3)-one+dxd
                        Sxd(4) = one-Sxd(5)-Sxd(3)
                        iter1min=3
                        iter1max=5
                    endif
                    if (dyd.le.half) then
                        Syd(2) = half * (dyd*dyd-dyd+quart)
                        Syd(4) = Syd(2) + dyd
                        Syd(3) = one-Syd(4)-Syd(2)
                        iter2min=2
                        iter2max=4
                    elseif(dyd.gt.half) then
                        Syd(3) = nineighth - thhalf*dyd + half*dyd*dyd
                        Syd(5) = Syd(3) - one + dyd
                        Syd(4) = one-Syd(5)-Syd(3)
                        iter2min=3
                        iter2max=5
                    endif
< #ifndef twoD
                    if (dzd.le.half) then
                        Szd(2) = half * (dzd*dzd-dzd+quart)
                        Szd(4) = Szd(2)+dzd
                        Szd(3) = one-Szd(4)-Szd(2)
                        iter3min=2
                       iter3max=4
                    {\tt elseif(dzd.gt.half)} \  \, {\tt then} \\
                       Szd(3) = nineighth - thhalf*dzd + half*dzd*dzd
Szd(5) = Szd(3)-one+dzd
                       Szd(4) = one-Szd(5)-Szd(3)
                       iter3min=3
                        iter3max=5
                    endif
< #endif
   ex0=0.
    ev0=0.
    ez0=0.
    bx0=0.
    by0=0.
    bz0=0.
```

```
< #ifndef twoD
    do iter3=iter3min,iter3max
       do iter2=iter2min,iter2max
             ! \ \texttt{lppp} = (\texttt{ip-3+iter1}) + \texttt{iy*}(\texttt{jp-3+iter2-1}) + \texttt{iz*}(\texttt{kp-3+iter3-1})
             !if (lppp.ge.1 .and. lppp.le.lot) then
                  print *, "out of range"
             !endif
                \verb|ex0=ex0+sum(ex_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)|
                  = y0 = y0 + sum(ey_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2)*Sxp(iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Sxp(iter3) 
                ez0=ez0+sum(ez_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)
                bx0=bx0+sum(bx_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,xp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)
                by0=by0+sum(by_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,xp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)
                bz0=bz0+sum(bz_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)
          !endif
<
       enddo
   enddo
< #else
   do iter2=iter2min,iter2max
       do iter1=iter1min.iter1max
          lpp=(ip-3+iter1)+iy*(jp-3+iter2-1)
          lpd=(ip-3+iter1)+iy*(jd-3+iter2-1)
          ldp=(id-3+iter1)+iy*(jp-3+iter2-1)
          ldd=(id-3+iter1)+iy*(jd-3+iter2-1)
<
          \verb|ex0=ex0+ex(ldp,1,1)*Sxd(iter1)*Syp(iter2)|\\
          ey0=ey0+ey(lpd,1,1)*Sxp(iter1)*Syd(iter2)
          ez0=ez0+ez(lpp,1,1)*Sxp(iter1)*Syp(iter2)
          bx0=bx0+bx(lpd,1,1)*Sxp(iter1)*Syd(iter2)
<
          \verb|by0=by0+by(ldp,1,1)*Sxd(iter1)*Syp(iter2)|\\
          bz0=bz0+bz(ldd,1,1)*Sxd(iter1)*Syd(iter2)
       enddo
   enddo
< #endif
    ex0=0.5*ex0*qm
    ey0=0.5*ey0*qm
    ez0=0.5*ez0*qm
   bx0=0.5*bx0*qm*cinv
   by0=0.5*by0*qm*cinv
   bz0=0.5*bz0*qm*cinv
    if(external_fields) then
       call get_external_fields(real(p(npr)%x,sprec),p(npr)%y,&
            p(npr)%z,ex_ext,ey_ext,ez_ext,bx_ext,by_ext,bz_ext)
       bx0=bx0+bx_ext*0.5*qm*cinv
       by0=by0+by_ext*0.5*qm*cinv
       bz0=bz0+bz_ext*0.5*qm*cinv
       ex0=ex0+ex_ext*0.5*qm
       ey0=ey0+ey_ext*0.5*qm
       ez0=ez0+ez_{ext}*0.5*qm
   endif
    !to be used later for synchrotron
   bx00=bx0
   by00=by0
    bz00=bz0
   ! First half electric acceleration, with relativity's gamma:
 #ifdef vav
   !Use Vay 2008 particle mover
    g=1./sqrt(1.+p(npr)\%u**2+p(npr)\%v**2+p(npr)\%w**2) \ !reciprocal \ of \ the \ Lorentz \ factor
   vx0=c*p(npr)%u*g !3-velocity of the particle
   vv0=c*p(npr)%v*g
   vz0=c*p(npr)%w*g
   u1=c*p(npr)%u+2.*ex0+vy0*bz0-vz0*by0 !uprime, taking into account
    !that cinv is already incorporated within B
   v1=c*p(npr)%v+2.*ey0+vz0*bx0-vx0*bz0
   w1=c*p(npr)%w+2.*ez0+vx0*by0-vy0*bx0
   !Lorentz factor for uprime
   ustar=cinv*(u1*bx0+v1*bv0+w1*bz0)
   sig=cinv*cinv*(c**2+u1**2+v1**2+w1**2)-(bx0**2+by0**2+bz0**2)
    g=1./sqrt(0.5*(sig+sqrt(sig**2+4.*(bx0**2+by0**2+bz0**2+ustar**2))))
    tx=bx0*g
   ty=by0*g
   tz=bz0*g
   f=1./(1.+tx**2+ty**2+tz**2)
   u0=f*(u1+(u1*tx+v1*ty+w1*tz)*tx+v1*tz-w1*ty)
```

```
v0=f*(v1+(u1*tx+v1*ty+w1*tz)*ty+w1*tx-u1*tz)
   w0=f*(w1+(u1*tx+v1*ty+w1*tz)*tz+u1*ty-v1*tx)
< #else
   !Use Boris algorithm
     First half electric acceleration, with Lorentz gamma:
   u0=c*p(npr)%u+ex0
   v0=c*p(npr)%v+ey0
   w0=c*p(npr)%w+ez0
   ! First half magnetic rotation, with Lorentz gamma:
   g=c/sqrt(c**2+u0**2+v0**2+w0**2)
   bx0=g*bx0
   by0=g*by0
   bz0=g*bz0
   f=2./(1.+bx0*bx0+by0*by0+bz0*bz0)
   u1=(u0+v0*bz0-w0*by0)*f
<
   v1 = (v0 + w0 * bx0 - u0 * bz0) * f
   w1 = (w0 + u0 * by0 - v0 * bx0) * f
   ! Second half mag. rot'n & el. acc'n:
   u0=u0+v1*bz0-w1*bv0+ex0
   v0 = v0 + w1 * bx0 - u1 * bz0 + ev0
   w0=w0+u1*by0-v1*bx0+ez0
< #endif
<
   !user stripe
   ! \\ following \ tamburrini, \ cooling \ is \ implemented \ at this point,
<
   !after the Lorentz push
       Get normalized 4-velocity:
<
   p(npr)%u=u0*cinv
   p(npr)%v=v0*cinv
   p(npr)%w=w0*cinv
   ! stripe user
   ! freeze particles, to verify the generation of the correct fields
   ! (the three lines above should also be commented out)
                         p(npr)%u=p(npr)%u
                          p(npr)%v=p(npr)%v
                          p(npr)%w=p(npr)%w
   ! end stripe user
      Position advance:
   g=c/sqrt(c**2+u0**2+v0**2+w0**2)
   p(npr)%x=p(npr)%x + p(npr)%u*g*c
   p(npr)%y=p(npr)%y + p(npr)%v*g*c
   p(npr)%z=p(npr)%z + p(npr)%w*g*c
< end subroutine mover_2ord
```

6.4 mover_3ord()

```
subroutine mover_3ord()
< subroutine mover_3ord(n1,n2,qm)
       implicit none
       ! dummy variables
       integer, intent(in) :: n2, n1
       real(sprec), intent(in) :: qm
       ! local variables
         integer :: iter1, iter2, iter3, iter1min, iter1max, iter2min, iter2max, iter3min, iter3max
         real, DIMENSION(6) :: Sxp,Syp,Sxd,Syd,Szp,Szd
<
       integer :: npr,1,n,ip,jp,kp,id,jd,kd
         integer :: lpp,lpd, ldp, ldd
<
         integer :: lppp
       \verb"real" dxp,dyp,dzp,dxd,dyd,dzd,f,g,ex0,ey0,ez0,bx0,by0,bz0"
       real u0,v0,w0,u1,v1,w1, cinv, g1, corrqm
<
       real qm0
         logical :: cond1, cond2, cond3, cond4
< !, xglob, yglob, gammawall, betawall, gamma, walloc
```

```
< !
        real vdriftx, vdrifty, gdrift, decrem
< !
        integer ::yes_gammacut
        real gammacut
< #ifdef vay
        real ustar, sig, tx, ty, tz, vx0, vy0, vz0
< #endif
          real bx_ext, by_ext, bz_ext, ex_ext, ey_ext, ez_ext
          real chival, threed
          real exsc, eysc, ezsc, bxsc, bysc, bzsc, v3x0, v3y0, v3z0
          real up, vp, wp, gampinv, ppinv, gamp, dragx, dragy, dragz, lfx, lfy, lfz, edotv, lsq
          \verb|real| bx00, by00, bz00, drag coeff, drag thresh, \verb|reduction| factor|
          integer redLL
          real gammathinv
<
          \verb"real,dimension"(\verb"mx,my,mz")::====p, ey_p, ez_p, bx_p, by_p, bz_p"
          ! primal grids
ex_p=0.5*(ex+cshift(ex,-1,dim=1))
          ey_p=0.5*(ey+cshift(ey,-1,dim=2))
          ez_p=0.5*(ez+cshift(ez,-1,dim=3))
          bx_p=0.5*(bx+cshift(bx,-1,dim=2))
          by_p=0.5*(by+cshift(by,-1,dim=1))
          bz_p=0.5*(0.5*(bz+cshift(bz,-1,dim=1))&
                +0.5*(cshift(bz,-1,dim=2)+cshift(cshift(bz,-1,dim=2),-1,dim=1)))
< !user stripe cooling</pre>
< redLL=1 ! if 1 then use reduced Landau Lifshits, otherwise Hededal (apart from 1/beta^2)</pre>
< dragthresh=1e-1 ! maximum differential change in momentum
   gammathinv=1./(1.+3.*delgam)
< !end user stripe cooling</pre>
< 1
        {\tt real\ pcosth,\ pphi,\ psinth,\ v0t,\ ut1,\ vt1,\ wt1,\ gam}
< !
        real ptx, pty, ptz
1
        cinv=1./c
<
        qm0=qm
        do n=n1,n2
                 ip=aint(p(npr)%x)
                 dxp=p(npr)%x-ip
                 jp=aint(p(npr)%y)
                 dyp=p(npr)%y-jp
                 kp=aint(p(npr)%z)
                   Sxp(:)=0.
                   Syp(:)=0.
                  id=aint(p(npr)%x-half)
                 dxd=p(npr)%x-half-id
                 jd=aint(p(npr)%y-half)
                 dyd=p(npr)%y-half-jd
                 kd=aint(p(npr)%z-half)
                   Sxd(:)=0.
                   Syd(:)=0.
< #ifndef twoD</pre>
                   dzp=p(npr)%z-kp
                   Szp(:)=0.
                   dzd=(p(npr)%z-half)-kd
                   Szd(:)=0.
< #endif
< !3 order form factor
< !----
<
      if (dxp.le.half) then
          Sxp(2)= negsixth*(dxp-one)*(dxp-one)*(dxp-one)
          Sxp(3) = twoth+half*(dxp-two)*dxp*dxp
<
          Sxp(5) = sixth *dxp*dxp*dxp
          Sxp(4) = one - Sxp(5) - Sxp(3) - Sxp(2)
<
          iter1min = 2
          iter1max = 5
      elseif (dxp.gt.half) then
          Sxp(5)=sixth*dxp*dxp*dxp
          Sxp(4)=twoth+half*(negone-dxp)*(one-dxp)*
          Sxp(2)=sixth*(one-dxp)*(one-dxp)*(one-dxp)
          Sxp(3) = one - Sxp(5) - Sxp(4) - Sxp(2)
          iter1min = 2
          iter1max = 5
       endif
       if (dyp.le.half) then
          Syp(2) = negsixth*(dyp-one)*(dyp-one)*(dyp-one)
```

```
Syp(3) = twoth+half*(dyp-two)*dyp*dyp
          Syp(5) = sixth *dyp*dyp*dyp
          Syp(4) = one - Syp(5) - Syp(3) - Syp(2)
          iter2min = 2
          iter2max = 5
     elseif (dyp.gt.half) then
          Syp(5)=sixth*dyp*dyp*dyp
          Syp(4)=twoth+half*(negone-dyp)*(one-dyp)*(one-dyp)
          Syp(2)=sixth*(one-dyp)*(one-dyp)*(one-dyp)
          Syp(3) = one - Syp(5) - Syp(4) - Syp(2)
          iter2min = 2
          iter2max = 5
      endif
< #ifndef twoD
       if (dzp.le.half) then
          Szp(2) = negsixth*(dzp-one)*(dzp-one)*(dzp-one)
          Szp(3) = twoth+half*(dzp-two)*dzp*dzp
          Szp(5) = sixth *dzp*dzp*dzp
          Szp(4) = one-Szp(5)-Szp(3)-Szp(2)
          iter3min = 2
         iter3max = 5
     elseif (dzp.gt.half) then
          Szp(5)=sixth*dzp*dzp*dzp
          Szp(2)=sixth*(one-dzp)*(one-dzp)*(one-dzp)
Szp(3)=one-Szp(5)-Szp(4)-Szp(2)
          iter3min = 2
          iter3max = 5
       endif
< #endif
       if (dxd.le.half) then
          Sxd(2)= negsixth*(dxd-one)*(dxd-one)*(dxd-one)
          Sxd(3) = twoth+half*(dxd-two)*dxd*dxd
          Sxd(5) = sixth *dxd*dxd*dxd
          Sxd(4) = one-Sxd(5)-Sxd(3)-Sxd(2)
          iter1min = 2
          iter1max = 5
     elseif (dxd.gt.half) then
          Sxd(5)=sixth*dxd*dxd*dxd
          Sxd(4)=twoth+half*(negone-dxd)*(one-dxd)*(one-dxd)
          Sxd(2)=sixth*(one-dxd)*(one-dxd)*(one-dxd)
          Sxd(3) = one - Sxd(5) - Sxd(4) - Sxd(2)
          iter1min = 2
          iter1max = 5
       endif
       if (dyd.le.half) then
          Syd(2) = negsixth*(dyd-one)*(dyd-one)*(dyd-one)
          Syd(3) = twoth+half*(dyd-two)*dyd*dyd
          Syd(5) = sixth *dyd*dyd*dyd
         Syd(4) = one-Syd(5)-Syd(3)-Syd(2)
          iter2min = 2
          iter2max = 5
     elseif (dyd.gt.half) then
        Syd(5)=sixth*dyd*dyd*dyd
          Syd(4)=twoth+half*(negone-dyd)*(one-dyd)*(one-dyd)
          Syd(2)=sixth*(one-dyd)*(one-dyd)*(one-dyd)
          Syd(3) = one - Syd(5) - Syd(4) - Syd(2)
          iter2min = 2
          iter2max = 5
      endif
 #ifndef twoD
      if (dzd.le.half) then
          Szd(2)= negsixth*(dzd-one)*(dzd-one)*(dzd-one)
          Szd(3) = twoth+half*(dzd-two)*dzd*dzd
          Szd(5) = sixth *dzd*dzd*dzd
         Szd(4) = one-Szd(5)-Szd(3)-Szd(2)
          iter3min = 2
         iter3max = 5
     elseif (dzd.gt.half) then
         Szd(5)=sixth*dzd*dzd*dzd
          Szd(4)=twoth+half*(negone-dzd)*(one-dzd)*(one-dzd)
          Szd(2)=sixth*(one-dzd)*(one-dzd)*(one-dzd)
          Szd(3) = one - Szd(5) - Szd(4) - Szd(2)
          iter3min = 2
          iter3max = 5
      endif
< #endif
   ex0=0.
   ey0=0.
   ez0=0.
   bx0=0.
   by0=0.
   bz0=0.
```

```
< #ifndef twoD
    do iter3=iter3min,iter3max
       do iter2=iter2min,iter2max
             !lppp=(ip-3+iter1)+iy*(jp-3+iter2-1)+iz*(kp-3+iter3-1)
             !if (lppp.ge.1 .and. lppp.le.lot) then
                  print *, "out of range"
                \verb|ex0=ex0+sum(ex_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)|
                ey0=ey0+sum(ey_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,xp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)
                ez0=ez0+sum(ez_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)
                bx0=bx0+sum(bx_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)
                by0=by0+sum(by_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,xp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)
                bz0=bz0+sum(bz_p(ip-3+iter1min:ip-3+iter1max,jp-3+iter2,kp-3+iter3)*Sxp(iter1min:iter1max))*Syp(iter2)*Szp(iter3)
       enddo
   enddo
< #else
    do iter2=iter2min,iter2max
      do iter1=iter1min.iter1max
          lpp=(ip-3+iter1)+iy*(jp-3+iter2-1)
          lpd=(ip-3+iter1)+iy*(jd-3+iter2-1)
          ldp=(id-3+iter1)+iy*(jp-3+iter2-1)
<
          ldd=(id-3+iter1)+iy*(jd-3+iter2-1)
          ex0=ex0+ex(ldp,1,1)*Sxd(iter1)*Syp(iter2)
          ey0=ey0+ey(lpd,1,1)*Sxp(iter1)*Syd(iter2)
          ez0=ez0+ez(lpp,1,1)*Sxp(iter1)*Syp(iter2)
          bx0=bx0+bx(lpd,1,1)*Sxp(iter1)*Syd(iter2)
          by0=by0+by(ldp,1,1)*Sxd(iter1)*Syp(iter2)
          bz0=bz0+bz(ldd,1,1)*Sxd(iter1)*Syd(iter2)
      enddo
   enddo
< #endif
    ex0=0.5*ex0*qm
    ey0=0.5*ey0*qm
    ez0=0.5*ez0*qm
   bx0=0.5*bx0*qm*cinv
   by0=0.5*by0*qm*cinv
   bz0=0.5*bz0*qm*cinv
   if(external_fields) then
       call get_external_fields(real(p(npr)%x,sprec),p(npr)%y,&
            p(npr)%z,ex_ext,ey_ext,ez_ext,bx_ext,by_ext,bz_ext)
      bx0=bx0+bx_ext*0.5*qm*cinv
      by0=by0+by_ext*0.5*qm*cinv
      bz0=bz0+bz_ext*0.5*qm*cinv
      ex0=ex0+ex_ext*0.5*qm
      ey0=ey0+ey_ext*0.5*qm
      ez0=ez0+ez_ext*0.5*qm
    !to be used later for synchrotron
    by00=by0
   bz00=bz0
       First half electric acceleration, with relativity's gamma:
 #ifdef vay
    !Use Vay 2008 particle mover
   g=1./\sqrt{1.+p(npr)}%u**2+p(npr)%u**2+p(npr)%v**2+p(npr)%w**2) !reciprocal of the Lorentz factor
    vx0=c*p(npr)%u*g !3-velocity of the particle
   vy0=c*p(npr)%v*g
    vz0=c*p(npr)%w*g
   u1=c*p(npr)%u+2.*ex0+vy0*bz0-vz0*by0 !uprime, taking into account
   !that cinv is already incorporated within B
    v1=c*p(npr)%v+2.*ey0+vz0*bx0-vx0*bz0
   w1=c*p(npr)%w+2.*ez0+vx0*by0-vy0*bx0
   !Lorentz factor for uprime
   ustar=cinv*(u1*bx0+v1*bv0+w1*bz0)
   sig=cinv*cinv*(c**2+u1**2+v1**2+w1**2)-(bx0**2+by0**2+bz0**2)
   g=1./sqrt(0.5*(sig+sqrt(sig**2+4.*(bx0**2+by0**2+bz0**2+ustar**2))))
   tx=bx0*g
   ty=by0*g
   tz=bz0*g
   f=1./(1.+tx**2+ty**2+tz**2)
    \verb"u0=f*(u1+(u1*tx+v1*ty+w1*tz)*tx+v1*tz-w1*ty)"
    v0=f*(v1+(u1*tx+v1*ty+w1*tz)*ty+w1*tx-u1*tz)
```

```
w0=f*(w1+(u1*tx+v1*ty+w1*tz)*tz+u1*ty-v1*tx)
 !Use Boris algorithm
       First half electric acceleration, with Lorentz gamma:
   u0=c*p(npr)%u+ex0
   v0=c*p(npr)%v+ey0
   w0=c*p(npr)%w+ez0
   ! First half magnetic rotation, with Lorentz gamma:
   g=c/sqrt(c**2+u0**2+v0**2+w0**2)
   bx0=g*bx0
   by0=g*by0
   bz0=g*bz0
   f=2./(1.+bx0*bx0+by0*by0+bz0*bz0)
   u1=(u0+v0*bz0-w0*by0)*f
   v1 = (v0 + w0 * bx0 - u0 * bz0) * f
   w1 = (w0 + u0 * by0 - v0 * bx0) * f
   ! Second half mag. rot'n & el. acc'n: u0=u0+v1*bz0-w1*by0+ex0
   v0=v0+w1*bx0-u1*bz0+ey0
<
   w0=w0+u1*by0-v1*bx0+ez0
< #endif
    !user stripe
    !following tamburrini, cooling is implemented at this point,
   !after the Lorentz push
       Get normalized 4-velocity:
   p(npr)%u=u0*cinv
   p(npr)%v=v0*cinv
<
   p(npr)%w=w0*cinv
   ! stripe user
<
   ! freeze particles, to verify the generation of the correct fields
    ! (the three lines above should also be commented out)
                         p(npr)%u=p(npr)%u
                          p(npr)%v=p(npr)%v
                          p(npr)%w=p(npr)%w
   ! end stripe user
   ! Position advance:
   g=c/sqrt(c**2+u0**2+v0**2+w0**2)
   p(npr)%x=p(npr)%x + p(npr)%u*g*c
   p(npr)%y=p(npr)%y + p(npr)%v*g*c
   p(npr)%z=p(npr)%z + p(npr)%w*g*c
< end subroutine mover_3ord
```

6.5 deposit_particles()

```
1358,1361c424,427
         maxx=mx-1.*(nghost/2)
         minx=1.*(nghost/2+1)
         maxy=my-1.*(nghost/2)
         miny=1.*(nghost/2+1)
         maxx=mx-2.
         minx=3.
         maxy=my-2.
         miny=3
1367,1368c433,434
         maxz=mz-1.*(nghostz/2)
         minz=1.*(nghostz/2+1)
         maxz=mz-2.
          minz=3.
1370,1371c436,437
         minz=1.*(nghostz/2+1)
         maxz=1.*(nghostz/2+1)+1
         minz=3.
          maxz= 6.-2.
```

The modifications are not tested with #define cleancur option used in the tristan-mp-pu-master version.

```
1377c443
< !#define cleancur
---
> #define cleancur
1379c445
```

```
< !#ifdef cleancur
> #ifdef cleancur
1382c448
< !#endif
> #endif
1391,1404c457,458
< #ifdef zzag
                                                   call zigzag(p(n1)%x,p(n1)%y,p(n1)%z,x0,y0,z0,in)
< #endif
< #ifdef dd1
                                                   call densdecomp_lord(p(n1)%x,p(n1)%y,p(n1)%z,x0,y0,z0,in)
< #endif
< #ifdef dd2
                                                   call densdecomp_2ord(p(n1)x,p(n1)y,p(n1)z,x0,y0,z0,in)
< #endif
< #ifdef dd3
                                             call densdecomp_3ord(p(n1)%x,p(n1)%y,p(n1)%z,x0,y0,z0,in)
< #endif
< !#ifdef findNaN
> !
                                             call zigzag(p(n1)\%x, p(n1)\%y, p(n1)\%z, x0, y0, z0, in)
> #ifdef findNaN
1406,1416c460,470
< 1
                     xt=p(n1)%x !hack -- this is needed for printout only
< 1
                      yt=p(n1)%y
<!
                      zt=p(n1)%z
< !
                      write(*,'(A,I7,A,3(I6,A),6(F8.4,A),3(I6,A))') "prb in ion dep, ind, proc, lap, rank: ",p(n1)%ind," ",p(n1)%proc," ",&
lap," ",rank," x=",p(n1)%x," y=",p(n1)%y," z=",p(n1)%z," u=",p(n1)%u," v=",&
    p(n1)%v," w=",p(n1)%w, " mx,y,z=",mx," ",my," ",mz
<!
<!
< !
<
<!
                                  x0=5.
<!
                                  y0=5.
< !
                                  z0=5.
---
                      xt=p(n1)%x !hack -- this is needed for printout only
                      yt=p(n1)%y
                      if(xt<0 .or. yt<0 .or. zt<0 .or. isnan(xt*yt*zt) .or. xt>mx-1.or.yt>my-1 ) then !.or.zt>mz-1) then !.or.zt>mz-1 | then !.or.
                                  write(*,'(A,I7,A,3(I6,A),6(F8.4,A),3(I6,A))') "prb in ion dep, ind, proc, lap, rank: ",p(n1)%ind," ",p(n1)%proc," ",&
lap," ",rank," x=",p(n1)%x," y=",p(n1)%y," z=",p(n1)%z," u=",p(n1)%u," v=",&
    p(n1)%v," w=",p(n1)%w, " mx,y,z=",mx," ",my," ",mz
                                   z0=5
1424,1425c478,479
                       endif
 < !#endif
                       endif
> #endif
```

The tristan-mp-pu-master version implements the zigzag current deposit in the subroutine deposit_particles(), but external to the zigzag subroutine defined in particles.F90(meaning, call zigzag(···) is commented out, and the full routine is copied afterward, with a few additional parts and slightly different notation). For the modified code, the external copy of zigzag is commented out, and is instead called with the zigzag subroutine.

```
1429,1452c483,506
          ! x1sp=x0
          ! x2sp=p(n1)%x
          ! v1sp=v0
          ! y2sp=p(n1)%y
          ! z1=z0
          ! z2=p(n1)%z
         ! i1=int(x1sp)
          ! i2=int(x2sp)
          ! j1=int(y1sp)
          ! i2=int(y2sp)
          ! k1=int(z1)
         ! k2=int(z2)
       ! xr=min(real(min(i1,i2)+1),max(real(max(i1,i2)),.5*(x1sp+x2sp)))
        ! yr=min(real(min(j1,j2)+1), max(real(max(j1,j2)),.5*(y1sp+y2sp)))
        ! zr=min(real(min(k1,k2)+1), max(real(max(k1,k2)), .5*(z1+z2)))
```

```
< ! #ifdef twoD
< ! #endif
            x1sp=x0
           x2sp=p(n1)%x
           y1sp=y0
           y2sp=p(n1)%y
         z1=z0
          z2=p(n1)%z
         i1=int(x1sp)
i2=int(x2sp)
j1=int(y1sp)
j2=int(y2sp)
k1=int(z1)
k2=int(z2)
        xr=min(real(min(i1,i2)+1), max(real(max(i1,i2)),.5*(x1sp+x2sp)))
         yr=min(real(min(j1,j2)+1),max(real(max(j1,j2)),.5*(y1sp+y2sp)))
zr=min(real(min(k1,k2)+1),max(real(max(k1,k2)),.5*(z1+z2)))
> #ifdef twoD
                   k1=1
                   k2 = 1
> #endif
1456,1543c510,597
        ! Fx1=-q*(xr-x1sp)
         ! Fy1=-q*(yr-y1sp)
        ! Fz1=-q*(zr-z1)
<
         ! Wx1=.5*(x1sp+xr)-i1
        ! Wy1=.5*(y1sp+yr)-j1
< ! #ifndef twoD
              Wz1=.5*(z1+zr)-k1
< ! #endif
         Wx2=.5*(x2sp+xr)-i2
< !
< !
         Wy2=.5*(y2sp+yr)-j2
< ! #ifndef twoD
< !
                   Wz2=.5*(z2+zr)-k2
< ! #endif
         ! Fx2=-q*(x2sp-xr)
         ! Fy2=-q*(y2sp-yr)
         ! Fz2=-q*(z2-zr)
< ! #ifdef twoD
                   Wz1=0
< ! #endif
   ! onemWx1=1.-Wx1
    ! onemWx2=1.-Wx2
   ! onemWy1=1.-Wy1
    ! onemWy2=1.-Wy2
    ! onemWz1=1.-Wz1
    ! onemWz2=1.-Wz2
< ! i1p1=i1+1
< ! i2p1=i2+1</pre>
< ! j1p1=j1+1
       j2p1=j2+1
< ! #ifndef twoD
< ! k1p1=k1+1
      k2p1=k2+1
< !
<! #endif
< ! #ifdef cleancur
< ! curx(i1,j1,k1)=curx(i1,j1,k1)+Fx1 * onemWy1 * onemWz1</pre>
      curx(i1,j1p1,k1)=curx(i1,j1p1,k1)+Fx1 * Wy1 * onemWz1
< !
< ! #ifndef twoD
< ! curx(i1,j1, k1p1)= curx(i1,j1, k1p1)+Fx1 * onemWy1 * Wz1
< ! curx(i1,j1p1,k1p1)= curx(i1,j1p1,k1p1)+Fx1 * Wy1 * Wz1</pre>
< ! #endif
< \ ! \quad \mathtt{curx(i2,j2,k2)} \mathtt{=} \mathtt{curx(i2,j2,k2)} \mathtt{+} \mathtt{Fx2} \ * \ \mathtt{onemWy2} \ * \ \mathtt{onemWz2}
      curx(i2,j2p1,k2)=curx(i2,j2p1,k2)+Fx2 * Wy2 * onemWz2
< ! #ifndef twoD
```

```
curx(i2,j2, k2p1)= curx(i2,j2, k2p1)+Fx2 * onemWy2* Wz2
      curx(i2, j2p1, k2p1) = curx(i2, j2p1, k2p1) + Fx2 * Wy2 * Wz2
< ! #endif
      cury(i1,j1,k1)=cury(i1,j1,k1)+Fy1 * onemWx1 * onemWz1
       cury(i1p1,j1,k1)=cury(i1p1,j1,k1)+Fy1 * Wx1 * onemWz1
  ! #ifndef twoD
<! cury(i1 ,j1,k1p1)= cury(i1 ,j1,k1p1)+Fy1 * onemWx1 * Wz1
<! cury(i1p1,j1,k1p1)= cury(i1p1,j1,k1p1)+Fy1 * Wx1 * Wz1</pre>
  ! #endif
    cury(i2,j2,k2)=cury(i2,j2,k2)+Fy2 * onemWx2 * onemWz2
      cury(i2p1,j2,k2)=cury(i2p1,j2,k2)+Fy2 * Wx2 * onemWz2
  ! #ifndef twoD
    cury(i2 ,j2,k2p1)= cury(i2 ,j2,k2p1)+Fy2 * onemWx2 * Wz2 cury(i2p1,j2,k2p1)= cury(i2p1,j2,k2p1)+Fy2 * Wx2 * Wz2
<! #endif
    ! curz(i1,j1,k1)=curz(i1,j1,k1)+ Fz1 * onemWx1 * onemWy1
! curz(i1p1,j1,k1)=curz(i1p1,j1,k1)+Fz1 * Wx1 * onemWy1
    ! curz(i1,j1p1,k1)=curz(i1,j1p1,k1)+Fz1 * onemWx1 * Wy1
    ! curz(i1p1,j1p1,k1)=curz(i1p1,j1p1,k1)+Fz1 * Wx1 * Wy1
    ! curz(i2,j2,k2)=curz(i2,j2,k2)+ Fz2 * onemWx2 * onemWy2
    ! curz(i2p1,j2,k2)=curz(i2p1,j2,k2)+ Fz2 * Wx2 * onemWy2
! curz(i2,j2p1,k2)=curz(i2,j2p1,k2)+ Fz2 * onemWx2 * Wy2
    ! curz(i2p1,j2p1,k2)=curz(i2p1,j2p1,k2)+ Fz2 * Wx2 * Wy2
< !#endif !cleancur
< enddo !m,n=1,ions
< !#define dontSKIP
< !#ifdef dontSKIP</pre>
< !
            pind(1:ions)=0
___
         Fx1=-q*(xr-x1sp)
        Fy1=-q*(yr-y1sp)
        Fz1=-q*(zr-z1)
         Wx1=.5*(x1sp+xr)-i1
         Wy1 = .5*(y1sp+yr)-j1
> #ifndef twoD
           Wz1=.5*(z1+zr)-k1
> #endif
         Wx2=.5*(x2sp+xr)-i2
         Wy2=.5*(y2sp+yr)-j2
> #ifndef twoD
                  Wz2=.5*(z2+zr)-k2
         Fx2=-q*(x2sp-xr)
         Fy2=-q*(y2sp-yr)
         Fz2=-q*(z2-zr)
> #ifdef twoD
                  Wz2=0
> #endif
   onemWx1=1.-Wx1
    onemWx2=1.-Wx2
    onemWy1=1.-Wy1
    onemWy2=1.-Wy2
    onemWz1=1.-Wz1
    onemWz2=1.-Wz2
    i1p1=i1+1
    i2p1=i2+1
   j1p1=j1+1
     j2p1=j2+1
> #ifndef twoD
   k1p1=k1+1
    k2p1=k2+1
> #endif
> #ifdef cleancur
    \texttt{curx(i1,j1,k1)} = \texttt{curx(i1,j1,k1)} + \texttt{Fx1} * \texttt{onemWy1} * \texttt{onemWz1}
    curx(i1,j1p1,k1)=curx(i1,j1p1,k1)+Fx1 * Wy1 * onemWz1
> #ifndef twoD
   curx(i1,j1, k1p1)= curx(i1,j1, k1p1)+Fx1 * onemWy1 * Wz1 curx(i1,j1p1,k1p1)= curx(i1,j1p1,k1p1)+Fx1 * Wy1 * Wz1
> #endif
```

```
curx(i2,j2,k2)=curx(i2,j2,k2)+Fx2 * onemWy2 * onemWz2
    curx(i2,j2p1,k2)=curx(i2,j2p1,k2)+Fx2 * Wy2 * onemWz2
> #ifndef twoD
  curx(i2,j2, k2p1)= curx(i2,j2, k2p1)+Fx2 * onemWy2* Wz2
    curx(i2,j2p1,k2p1) = curx(i2,j2p1,k2p1)+Fx2 * Wy2 * Wz2
   cury(i1,j1,k1)=cury(i1,j1,k1)+Fy1 * onemWx1 * onemWz1
    cury(i1p1,j1,k1)=cury(i1p1,j1,k1)+Fy1 * Wx1 * onemWz1
> #ifndef twoD
   cury(i1 ,j1,k1p1)= cury(i1 ,j1,k1p1)+Fy1 * onemWx1 * Wz1
cury(i1p1,j1,k1p1)= cury(i1p1,j1,k1p1)+Fy1 * Wx1 * Wz1
> #endif
   cury(i2,j2,k2)=cury(i2,j2,k2)+Fy2 * onemWx2 * onemWz2
    cury(i2p1,j2,k2)=cury(i2p1,j2,k2)+Fy2 * Wx2 * onemWz2
> #ifndef twoD
   cury(i2 ,j2,k2p1)= cury(i2 ,j2,k2p1)+Fy2 * onemWx2 * Wz2 cury(i2p1,j2,k2p1)= cury(i2p1,j2,k2p1)+Fy2 * Wx2 * Wz2
> #endif
    \verb"curz"(i1,j1,k1) = \verb"curz"(i1,j1,k1) + Fz1 * onemWx1 * onemWy1"
    curz(i1p1,j1,k1)=curz(i1p1,j1,k1)+Fz1 * Wx1 * onemWy1
   curz(i1,j1p1,k1)=curz(i1,j1p1,k1)+Fz1 * onemWx1 * Wy1
curz(i1p1,j1p1,k1)=curz(i1p1,j1p1,k1)+Fz1 * Wx1 * Wy1
    curz(i2,j2,k2)=curz(i2,j2,k2)+Fz2 * onemWx2 * onemWy2
    curz(i2p1,j2,k2)=curz(i2p1,j2,k2)+ Fz2 * Wx2 * onemWy2
    curz(i2,j2p1,k2)=curz(i2,j2p1,k2)+ Fz2 * onemWx2 * Wy2
    curz(i2p1,j2p1,k2)=curz(i2p1,j2p1,k2)+ Fz2 * Wx2 * Wy2
> #endif !cleancur
           enddo !m,n=1,ions
> #define dontSKIP
> #ifdef dontSKIP
          pind(1:ions)=0
1570,1572c624,626
          \hbox{if(periodicz.eq.0.and. in) then}\\
              in=(p(n1)\%z+mzcum .gt. z1in) .and. (p(n1)\%z+mzcum .lt. z2in)
           endif
___
                 if(periodicz.eq.0 .and. in) then
                          in=(p(n1)\%z+mzcum .gt. z1in) .and. (p(n1)\%z+mzcum .lt. z2in)
1576,1614c630,668
          if (.not. in) then
                                                            !imp
             perx=0
                                                            !imp
             pery=0
                                                            !imp
              perz=0
                                                            !imp
           endif
                                                            !imp
           ! to send to another processor
           if (perx .ne. 0 .and. in .and. sizex .ne. 1) then !imp
              in=.false.
              pery=0
              perz=0
                                                                 !imp
          endif
                                                                !imp
           ! assume non-uniform mx
          if(perx .lt. 0 .and. sizex .ne. 1) then
              ! minus rank (-x direction)
              i1=(rank/sizex)*sizex + modulo(rank-1, sizex)
              perx=-(mxl(i1+1)-1.*nghost)
           endif
<
          p(n1)%x=p(n1)%x-perx
                                                              !imp
           ! to send to another processor
           if(pery .ne. 0 .and. in .and. sizey .ne. 1) then
                                                                   !imp
<
              in=.false.
                                                                   !imp
              perx=0
                                                                   !imp
              perz=0
                                                                   !imp
           endif
                                                                   !imp
           ! assume non-uniform my
           if(pery .lt. 0 .and. sizey .ne. 1) then
                                                                                                                  !imp
                            (-y direction)
              ! left rank
                                                                                                                  !imp
                                   j1=modulo((rank/sizex - 1), sizey)*sizex + modulo(rank, sizex)
                                                                                                         !imp
              j1=modulo(rank/sizex - 1,sizey)*sizex+rank/(sizex*sizey)*(sizex*sizey) &
                                                                                                           !imp
                                                                                                           !imp
                  + modulo(rank, sizex)
                                                                                                                  !imp
              pery=-(myl(j1+1)-1.*nghost)
<
           endif
          p(n1)%y=p(n1)%y-pery
```

```
if(.not. in) then
                                                                                                         perx=0
                                                                                                          pery=0
                                                                                                          perz=0
                                                                       ! to send to another processor if(perx .ne. 0 .and. in .and. sizex .ne. 1) then
                                                                                                          in=.false.
                                                                                                         pery=0
                                                                                                          perz=0
                                                                       endif
                                                                        ! assume non-uniform mx
                                                                      if(perx .lt. 0 .and. sizex .ne. 1) then
    ! minus rank (-x direction)
                                                                                                          i1=(rank/sizex)*sizex + modulo(rank-1, sizex)
                                                                                                          perx=-(mxl(i1+1)-5.)
                                                                       endif
                                                                       p(n1)%x=p(n1)%x-perx
                                                                        ! to send to another processor % \left( 1\right) =\left( 1\right) \left( 1\right) \left
                                                                       if(pery .ne. 0 .and. in .and. sizey .ne. 1) then
                                                                                                          in=.false.
                                                                                                          perx=0
                                                                                                         perz=0
                                                                       endif
                                                                       ! assume non-uniform my
                                                                       if(pery .1t. 0 .and. sizey .ne. 1) then
                                                                                                          ! left rank
                                                                                                                                                                           (-y direction)
                                                                                                          j1=modulo((rank/sizex - 1),sizey)*sizex + modulo(rank,sizex)
j1=modulo(rank/sizex - 1,sizey)*sizex+rank/(sizex*sizey)*(sizex*sizey) &
                                                                                                                                            + modulo(rank, sizex)
                                                                                                          pery=-(myl(j1+1)-5.)
                                                                       endif
                                                                       p(n1)\%y=p(n1)\%y-pery
1618,1629c672,683
                                        if(perz .ne. 0 .and. in ) then
                                                         in=.false.
                                                         perx=0
                                                         pery=0
                                             endif
                                             ! assume non-uniform mz
                                             if(perz .lt. 0) then
                                                           ! down rank
                                                                                                                                            (-z direction)
                                                          k1=modulo(rank/(sizex*sizey) - 1,sizez)*(sizex*sizey) + &
                                                                               modulo(rank,sizex*sizey)
                                                         perz=-(mzl(k1+1)-1.*nghostz)
                                             endif
                                                                       if(perz .ne. 0 .and. in ) then
                                                                                                          in=.false.
                                                                                                          perx=0
                                                                                                          pery=0
                                                                       endif
                                                                        ! assume non-uniform mz
                                                                       if(perz .lt. 0) then
                                                                                                           ! down rank
                                                                                                                                                                                (-z direction)
                                                                                                          k1=modulo(rank/(sizex*sizey) - 1,sizez)*(sizex*sizey) + &
                                                                                                                                 modulo(rank,sizex*sizey)
                                                                                                          perz=-(mzl(k1+1)-5.)
                                                                       endif
1705c759
< !#endif !dontSKIP</pre>
> #endif !dontSKIP
1728c782
< !#ifdef findNaN
> #ifdef findNaN
1730,1740c784,794
< !
                                  xt=p(n1)%x !hack -- this is needed for printout only
<!
                                   yt=p(n1)%y
< 1
                                   zt=p(n1)%z
                                  if(xt<0 .or. yt<0 .or. zt<0 .or. isnan(xt*yt*zt) .or. xt>mx-1.or.yt>my-1 ) then !.or.zt>mz-1) then
write(*,'(A,17,A,3(16,A),6(F8.4,A),3(16,A))') "prb in lec dep, ind, proc, lap, rank: ",p(n1)%ind," ",p(n1)%proc," ",&
lap," ",rank," x=",p(n1)%x," y=",p(n1)%y," z=",p(n1)%z," u=",p(n1)%u," v=",&
p(n1)%v," w=",p(n1)%w, " mx,y,z=",mx," ",my," ",mz
<!
< 1
< !
< !
<!
                                                     x0=5.
```

```
y0=5.
< !
< !
                                z_0=5.
---
                     xt=p(n1)%x
                                                     !hack -- this is needed for printout only
                     yt=p(n1)%y
                     zt=p(n1)%z
                      if(xt<0 \text{ .or. } yt<0 \text{ .or. } zt<0 \text{ .or. } isnan(xt*yt*zt) \text{ .or. } xt>mx-1.or.yt>my-1 \text{ ) then } !.or.zt>mz-1) \text{ t
                                write(*,'(A,17,A,3(16,A),6(F8.4,A),3(16,A))') "prb in lec dep, ind, proc, lap, rank: ",p(n1)%ind," ",p(n1)%proc," ",&
lap," ",rank," x=",p(n1)%x," y=",p(n1)%y," z=",p(n1)%z," u=",p(n1)%u," v=",&
    p(n1)%v," w=",p(n1)%w, " mx,y,z=",mx," ",my," ",mz
                                x0=5.
                                y0=5.
                                z_0=5.
1748,1761c802
                    endif
< !
< !#endif
< #ifdef zzag</pre>
                                           call zigzag(p(n1)%x,p(n1)%y,p(n1)%z,x0,y0,z0,in)
< #endif
< #ifdef dd1
                                                call densdecomp_lord(p(n1)x,p(n1)y,p(n1)z,x0,y0,z0,in)
< #endif
< #ifdef dd2
                                                call densdecomp_2ord(p(n1)x,p(n1)y,p(n1)z,x0,y0,z0,in)
< #endif
< #ifdef dd3
                                           call densdecomp_3ord(p(n1)%x,p(n1)%y,p(n1)%z,x0,y0,z0,in)
                     endif
1763a805,807
> !
                                           call zigzag(p(n1)\%x,p(n1)\%y,p(n1)\%z,x0,y0,z0,in)
1765,1788c809,832
                            x1sp=x0
< 1
                             x2sp=p(n1)%x
< !
                             y1sp=y0
< !
                            y2sp=p(n1)%y
< !
                             z1=z0
< !
                             z2=p(n1)%z
< !
                             i1=int(x1sp)
< !
                             i2=int(x2sp)
                             j1=int(y1sp)
                             j2=int(y2sp)
                             k1=int(z1)
< !
                            k2=int(z2)
                     xr=min(real(min(i1,i2)+1), max(real(max(i1,i2)),.5*(x1sp+x2sp)))
                    yr=min(real(min(j1,j2)+1), max(real(max(j1,j2)), .5*(y1sp+y2sp)))
                     zr=min(real(min(k1,k2)+1),max(real(max(k1,k2)),.5*(z1+z2)))
< !
< !#ifdef twoD</pre>
                                           k1=1
< !
                                           k2=1
< !#endif
                          x1sp=x0
                          x2sp=p(n1)%x
                          v1sp=v0
                          y2sp=p(n1)%y
                          z1 = z0
                          z2=p(n1)%z
                          i1=int(x1sp)
                          i2=int(x2sp)
                          j1=int(y1sp)
                           j2=int(y2sp)
                          k1=int(z1)
                          k2=int(z2)
                     xr=min(real(min(i1,i2)+1), max(real(max(i1,i2)),.5*(x1sp+x2sp)))
                     yr=min(real(min(j1,j2)+1), max(real(max(j1,j2)),.5*(y1sp+y2sp)))
                     zr=min(real(min(k1,k2)+1), max(real(max(k1,k2)), .5*(z1+z2)))
> #ifdef twoD
                                           k1=1
                                           k2 = 1
> #endif
```

```
1792,1833c836,877
        Fx1=-q*(xr-x1sp)
        Fy1=-q*(yr-y1sp)
< !
        Fz1=-q*(zr-z1)
        Wx1=.5*(x1sp+xr)-i1
      Wy1=.5*(y1sp+yr)-j1
< !#ifndef twoD
        Wx2=.5*(x2sp+xr)-i2
      Wy2=.5*(y2sp+yr)-j2
< !
< !#ifndef twoD</pre>
                 Wz2=.5*(z2+zr)-k2
< !#endif
< !
        Fx2=-q*(x2sp-xr)
      Fy2=-q*(y2sp-yr)
Fz2=-q*(z2-zr)
< !
< !
< !#ifdef twoD</pre>
                  Wz1=0
< 1
< !
                  Wz2=0
< !#endif
    ! onemWx1=1.-Wx1
    ! onemWx2=1.-Wx2
<
   ! onemWy1=1.-Wy1
   ! onemWy2=1.-Wy2
! onemWz1=1.-Wz1
   ! onemWz2=1.-Wz2
<! i1p1=i1+1
<! i2p1=i2+1
<! j1p1=j1+1
<!! j2p1=i2+1</pre>
< !
       j2p1=j2+1
< ! #ifndef twoD
< ! k1p1=k1+1
< ! k2p1=k2+1</pre>
< ! #endif
         Fx1=-q*(xr-x1sp)
       Fy1=-q*(yr-y1sp)
Fz1=-q*(zr-z1)
        Wx1=.5*(x1sp+xr)-i1
        Wy1=.5*(y1sp+yr)-j1
> #ifndef twoD
          Wz1=.5*(z1+zr)-k1
> #endif
        Wx2=.5*(x2sp+xr)-i2
        Wy2=.5*(y2sp+yr)-j2
> #ifndef twoD
                 Wz2=.5*(z2+zr)-k2
> #endif
        Fx2=-q*(x2sp-xr)
Fy2=-q*(y2sp-yr)
Fz2=-q*(z2-zr)
> #ifdef twoD
                  Wz1=0
                  Wz2=0
> #endif
    onemWx1=1.-Wx1
    onemWx2=1.-Wx2
    onemWy1=1.-Wy1
    onemWy2=1.-Wy2
    onemWz1=1.-Wz1
    onemWz2=1.-Wz2
    i1p1=i1+1
    i2p1=i2+1
    j1p1=j1+1
    j2p1=j2+1
> #ifndef twoD
   k1p1=k1+1
   k2p1=k2+1
```

```
> #endif
1835c879
< !#ifdef cleancur
> #ifdef cleancur
1840.1873c884.917
< ! curx(i1,j1,k1)=curx(i1,j1,k1)+Fx1 * onemWy1 * onemWz1</pre>
     curx(i1,j1p1,k1)=curx(i1,j1p1,k1)+Fx1 * Wy1 * onemWz1
< !#ifndef twoD
< ! curx(i1,j1, k1p1)= curx(i1,j1, k1p1)+Fx1 * onemWy1 * Wz1</pre>
<! curx(i1,j1p1,k1p1) = curx(i1,j1p1,k1p1) +Fx1 * Wy1</pre>
< !#endif
< ! curx(i2,j2,k2)=curx(i2,j2,k2)+Fx2 * onemWy2 * onemWz2</pre>
    curx(i2,j2p1,k2)=curx(i2,j2p1,k2)+Fx2 * Wy2 * onemWz2
< !#ifndef twoD
< ! curx(i2,j2, k2p1) = curx(i2,j2, k2p1) + Fx2 * onemWy2* Wz2</pre>
    curx(i2,j2p1,k2p1)= curx(i2,j2p1,k2p1)+Fx2 * Wy2
< !#endif
< ! cury(i1,j1,k1)=cury(i1,j1,k1)+Fy1 * onemWx1 * onemWz1</pre>
< \ ! \ \ cury(i1p1,j1,k1) = cury(i1p1,j1,k1) + Fy1 \ * \ Wx1 \ * \ onemWz1
< !#ifndef twoD
< ! cury(i1 ,j1,k1p1)= cury(i1 ,j1,k1p1)+Fy1 * onemWx1 * Wz1
< ! cury(i1p1,j1,k1p1)= cury(i1p1,j1,k1p1)+Fy1 * Wx1 * Wz1</pre>
< !#endif
< \ ! \quad \mathtt{cury}(\mathtt{i2},\mathtt{j2},\mathtt{k2}) \mathtt{=} \mathtt{cury}(\mathtt{i2},\mathtt{j2},\mathtt{k2}) \mathtt{+} \mathtt{Fy2} \ * \ \mathtt{onemWx2} \ * \ \mathtt{onemWx2}
< ! cury(i2p1,j2,k2)=cury(i2p1,j2,k2)+Fy2 * Wx2</pre>
                                                              * onemWz2
< !#ifndef twoD
< \ ! \ \text{cury(i2} \ , \text{j2,k2p1)= cury(i2} \ , \text{j2,k2p1)+Fy2} \ * \ \text{onemWx2} \ * \ \text{Wz2}
< ! cury(i2p1,j2,k2p1) = cury(i2p1,j2,k2p1) + Fy2 * Wx2</pre>
< !#endif
< ! curz(i1,j1,k1)=curz(i1,j1,k1)+ Fz1 * onemWx1 * onemWy1</pre>
< ! curz(i1p1,j1,k1)=curz(i1p1,j1,k1)+Fz1 * Wx1 * onemWy1</pre>
    curz(i1,j1p1,k1)=curz(i1,j1p1,k1)+Fz1 * onemWx1 * Wy1
< ! curz(i1p1,j1p1,k1)=curz(i1p1,j1p1,k1)+Fz1 * Wx1 * Wy1</pre>
    curz(i2, j2, k2) = curz(i2, j2, k2) + Fz2 * onemWx2 * onemWy2
< ! curz(i2p1,j2,k2)=curz(i2p1,j2,k2)+ Fz2 * Wx2 * onemWy2</pre>
< ! curz(i2,j2p1,k2)=curz(i2,j2p1,k2)+ Fz2 * onemWx2 * Wy2
< ! curz(i2p1,j2p1,k2)=curz(i2p1,j2p1,k2)+ Fz2 * Wx2 * Wy2</pre>
    curx(i1,j1,k1)=curx(i1,j1,k1)+Fx1 * onemWy1 * onemWz1
    curx(i1,j1p1,k1)=curx(i1,j1p1,k1)+Fx1 * Wy1 * onemWz1
    curx(i1,j1,
                    k1p1)= curx(i1,j1, k1p1)+Fx1 * onemWy1 * Wz1
    curx(i1,j1p1,k1p1)= curx(i1,j1p1,k1p1)+Fx1 * Wy1 * Wz1
    curx(i2,j2,k2)=curx(i2,j2,k2)+Fx2 * onemWy2 * onemWz2
    curx(i2,j2p1,k2)=curx(i2,j2p1,k2)+Fx2 * Wy2 * onemWz2
  curx(i2,j2, k2p1)= curx(i2,j2, k2p1)+Fx2 * onemWy2* Wz2
    curx(i2,j2p1,k2p1) = curx(i2,j2p1,k2p1) + Fx2 * Wy2
    cury(i1, j1, k1) = cury(i1, j1, k1) + Fy1 * onemWx1 * onemWz1
    cury(i1p1,j1,k1)=cury(i1p1,j1,k1)+Fy1 * Wx1 * onemWz1
  #ifndef twoD
    cury(i1 ,j1,k1p1)= cury(i1 ,j1,k1p1)+Fy1 * onemWx1 * Wz1
cury(i1p1,j1,k1p1)= cury(i1p1,j1,k1p1)+Fy1 * Wx1 * Wz1
> #endif
   \operatorname{cury}(i2,j2,k2) = \operatorname{cury}(i2,j2,k2) + \operatorname{Fy2} * \operatorname{onemWx2} * \operatorname{onemWz2}
    cury(i2p1,j2,k2)=cury(i2p1,j2,k2)+Fy2 * Wx2 * onemWz2
> #ifndef twoD
    cury(i2 ,j2,k2p1)= cury(i2 ,j2,k2p1)+Fy2 * onemWx2 * Wz2
cury(i2p1,j2,k2p1)= cury(i2p1,j2,k2p1)+Fy2 * Wx2 * Wz2
> #endif
    curz(i1,j1,k1)=curz(i1,j1,k1)+ Fz1 * onemWx1 * onemWy1
    curz(i1p1,j1,k1)=curz(i1p1,j1,k1)+Fz1 * Wx1 * onemWy1
    curz(i1,j1p1,k1)=curz(i1,j1p1,k1)+Fz1 * onemWx1 * Wy1
    curz(i1p1,j1p1,k1)=curz(i1p1,j1p1,k1)+Fz1 * Wx1 * Wy1 curz(i2,j2,k2)=curz(i2,j2,k2)+ Fz2 * onemWx2 * onemWy2
    curz(i2p1,j2,k2)=curz(i2p1,j2,k2)+ Fz2 * Wx2 * onemWy2
    curz(i2,j2p1,k2)=curz(i2,j2p1,k2)+ Fz2 * onemWx2 * Wy2
    curz(i2p1,j2p1,k2)=curz(i2p1,j2p1,k2)+ Fz2 * Wx2 * Wy2
1876c920
< !#endif !cleancur</pre>
> #endif !cleancur
1878,1879c922,923
< !107 continue
< enddo !n=1,lecs
> 107 continue
    enddo !n=1,lecs
```

```
1935c979
                        perx=-(mxl(i1+1)-1.*nghost)
                        perx=-(mxl(i1+1)-5.)
1953c996
                        pery=-(myl(j1+1)-1.*nghost)
___
                        pery=-(myl(j1+1)-5.)
1956c999
                p(n1)%y=p(n1)%y-pery
                p(n1)%y=p(n1)%y-pery
1970c1013
                        perz=-(mzl(k1+1)-1.*nghostz)
                        perz = -(mzl(k1+1)-5.)
2022d1064
2032d1073
             !print *, "discarding", pind(n), n, p(n)%x, p(n)%y, p(n)%z, lecs, lecs0, lap, rank
```

7 filter.F90

168c164

7.1 apply_filter1_opt()

```
29.30c29.30
        istr=nghost/2+1
<
        ifin=mx-(nghost/2+1)
        istr=2 +1
        ifin=mx-1-2
73,74c73
                        !call copy_layrx1_opt(curx,cury,curz,mx,my,mz,2,mx-3,mx-2,3)
                          \verb|call copy_layrx1_opt(curx,cury,curz,mx,my,mz,nghost/2,mx-(nghost/2+1),mx-(nghost/2),(nghost/2+1)|\\
___
                        call copy_layrx1_opt(curx,cury,curz,mx,my,mz,2,mx-3,mx-2,3)
77c76
                        call copy_layrx2_opt(curx,cury,curz,mx,my,mz,nghost/2,mx-(nghost/2+1),mx-(nghost/2),(nghost/2+1))
---
                        call copy_layrx2_opt(curx,cury,curz,mx,my,mz,2,mx-3,mx-2,3)
82,83c81
                        !call copy_layry1_opt(curx,cury,curz,mx,my,mz,2,my-3,my-2,3)
                          call copy_layry1_opt(curx,cury,curz,mx,my,mz,nghost/2,my-(nghost/2+1),my-nghost/2,(nghost/2+1))
---
                        call copy_layry1_opt(curx,cury,curz,mx,my,mz,2,my-3,my-2,3)
86,87c84
                        !call copy_layry2_opt(curx,cury,curz,mx,my,mz,2,my-3,my-2,3)
                          call copy_layry2_opt(curx,cury,curz,mx,my,mz,nghost/2,my-(nghost/2+1),my-nghost/2,(nghost/2+1))
                        call copy_layry2_opt(curx,cury,curz,mx,my,mz,2,my-3,my-2,3)
92,93c89
                                 !call copy_layrz1_opt(curx,cury,curz,mx,my,mz,2,mz-3,mz-2,3)
                                  call copy_layrz1_opt(curx,cury,curz,mx,my,mz,nghostz/2,mz-(nghostz/2+1),mz-nghostz/2,nghostz/2+1)
___
                                  call copy_layrz1_opt(curx,cury,curz,mx,my,mz,2,mz-3,mz-2,3)
97c93
                                 call copy_layrz2_opt(curx,cury,curz,mx,my,mz,nghostz/2,mz-(nghostz/2+1),mz-nghostz/2,nghostz/2+1)
<
                                 call copy_layrz2_opt(curx,cury,curz,mx,my,mz,2,mz-3,mz-2,3)
102c98
                do k=nghostz/2+1,mz-(nghostz/2+1)
<
                do k=3, mz-3
106c102
                do j=nghost/2+1,my-(nghost/2+1)
<
                do j=3, my-3
128c124
<
                do k=(nghostz/2+1),mz-(nghostz/2+1)
                do k=3.mz-3
132c128
                        do j=(nghost/2+1), my-(nghost/2+1)
<
---
                        do j=3,my-3
141c137
                do k=(nghostz/2+1), mz-(nghostz/2+1)
                do k=3.mz-3
145c141
                do j=(nghost/2+1), my-(nghost/2+1)
<
---
                do j=3,my-3
```

```
do k=(nghostz/2+1),mz-(nghostz/2+1)
                do k=3, mz-3
172c168
                        do j=nghost/2+1,my-(nghost/2+1)
                        do j=3,my-3
182c178
                do k=(nghostz/2+1),mz-(nghostz/2+1)
                do k=3, mz-3
186c182
                do j=nghost/2+1,my-nghost/2+1
                do j=3, my-3
207c203
                do k=(nghostz/2+1),mz-(nghostz/2+1)
                do k=3, mz-3
211c207
                        do j=nghost/2+1,my-nghost/2+1
---
                        do j=3,my-3
```

8 optimized_filters.F90

The option Dfilter2 is undocumented: ghost cell modifications are untested with filter2 (also filter3).

8.1 apply_filter2_opt()

8.2 apply_filter2_copy_opt()

8.3 filter_x()

8.4 chunk_filter()

```
1003,1004c1003,1004
                istr=nghost/2+1
                ifin=mx-(nghost/2+1)
                istr=3
                ifin=mx-3
1018,1019c1018,1019
                jstr=nghost/2+1
<
                jfin=my-(nghost/2+1)
                ifin=mv-3
1023,1024c1023,1024
                kstr=nghostz/2+1
                kfin=mz-(nghostz/2+1) !2,mz-1 !3,mz-3
<
                kfin=mz-3 !2,mz-1 !3,mz-3
1036,1042c1036,1042
                num_x_chunks = (mx-nghost)/x_chunk_len
num_y_chunks = (my-nghost)/y_chunk_len
                num_z_chunks = (mz-nghostz)/z_chunk_len
<
<
                last_x_size = (mx-nghost) - num_x_chunks*x_chunk_len
last_y_size = (my-nghost) - num_y_chunks*y_chunk_len
<
                last_z_size = (mz-nghostz) - num_z_chunks*z_chunk_len
<
                num_x_chunks = (mx-5)/x_chunk_len
num_y_chunks = (my-5)/y_chunk_len
>
                num_z_chunks = (mz-5)/z_chunk_len
                last_x_size = (mx-5) - num_x_chunks*x_chunk_len
last_y_size = (my-5) - num_y_chunks*y_chunk_len
last_z_size = (mz-5) - num_z_chunks*z_chunk_len
1077,1080c1077,1079
                                                                                 =xghost(:ntimes,(nghost/2+1)+(j-1)&
                                                                                      *y_chunk_len:(nghost/2+1)+ j*y_chunk_len-1,&
                                                                                      (nghostz/2+1)+(k-1)&
                                                                                      *z_chunk_len:(nghostz/2+1)+k*z_chunk_len-1)
___
                                                                                 =xghost(:ntimes,3+(j-1)*y_chunk_len:3+ &
                                                                                  j*y_chunk_len-1,3+(k-1)*z_chunk_len:3+ &
                                                                                 k*z_chunk_len-1)
1084,1087c1083,1086
                                                                                 = cur((nghost/2+1)+(i-1)&
                                                                                     *x_chunk_len-ntimes:(nghost/2+1)+(i-1)*x_chunk_len-1,&
                                                                                      (nghost/2+1)+(j-1)*y_chunk_len:(nghost/2+1)+j*y_chunk_len-1,&
                                                                                      (nghost/2+1)+(k-1)*z_chunk_len:(nghostz/2+1)+k*z_chunk_len-1)
                                                                                 =cur(3+(i-1)*x_chunk_len-ntimes:3+ &
                                                                                  (i-1)*x_chunk_len-1,3+(j-1)*y_chunk_len:3+ &
                                                                                  j*y_chunk_len-1,3+(k-1)*z_chunk_len:3+ &
                                                                                 k*z_chunk_len-1)
1092,1097c1091
                                                                                 chunk(ntimes+x_chunk_len+1:,&
                                                                                                 ntimes+1:ntimes+y_chunk_len,&
                                                                                                  ntimes+1:ntimes+z_chunk_len) &
                                                                                                  =xghost(ntimes+1:,&
                                                                                                  (\verb"nghost/2+1") + (\verb"j-1") * \verb"y_chunk_len" : (\verb"nghost/2+1") + \verb"j*y_chunk_len" - 1, \& 
                                                                                                  (nghostz/2+1)+(k-1)*z_chunk_len:(nghostz/2+1)+k*z_chunk_len-1)
                                                                                 chunk(ntimes+x_chunk_len+1:,ntimes+1:ntimes+y_chunk_len,ntimes+1:ntimes+z_chunk_len) ...
1099,1104c1093
                                                                                 chunk(ntimes+x chunk len+1:,&
<
                                                                                                  ntimes+1:ntimes+y_chunk_len,&
                                                                                                  ntimes+1:ntimes+z chunk len)&
                                                                                                  = cur((nghost/2+1)+i*x_chunk_len:(nghost/2+1)+i*x_chunk_len+ntimes-1,&(nghost/2+1)+(j-1)*y_chunk_len:(nghost/2+1)+j*y_chunk_len-1,&
<
                                                                                                  (nghostz/2+1)+(k-1)*z_chunk_len:(nghostz/2+1)+k*z_chunk_len-1)
<
                                                                                 chunk(ntimes+x_chunk_len+1:,ntimes+1:ntimes+y_chunk_len,ntimes+1:ntimes+z_chunk_len) ...
1109,1112c1098
                                                                                 chunk(ntimes+1:ntimes+x_chunk_len,:ntimes,&
                                                                                                  ntimes+1:ntimes+z_chunk_len)&
<
                                                                                                  =yghost((nghost/2+1)+(i-1)*x_chunk_len:(nghost/2+1)+i*x_chunk_len-1,&
<
                                                                                                  : \texttt{ntimes} \texttt{,} (\texttt{nghostz/2+1}) + (\texttt{k-1}) * \texttt{z\_chunk\_len} : (\texttt{nghostz/2+1}) + \texttt{k*z\_chunk\_len-1})
                                                                                 chunk(ntimes+1:ntimes+x chunk len.:ntimes.ntimes+1:ntimes+z chunk len) ...
1114,1118c1100
                                                                                  \verb|chunk(ntimes+1:ntimes+x_chunk_len,:ntimes,\&
                                                                                                  \verb|ntimes+1:ntimes+z_chunk_len| \&
                                                                                                  =cur((nghost/2+1)+(i-1)*x_chunk_len:(nghost/2+1)+i*x_chunk_len-1,&
<
                                                                                                  (nghost/2+1) + (j-1)*y\_chunk\_len-ntimes: (nghost/2+1) + (j-1)*y\_chunk\_len-1, \& and beta + (j-1)*y\_chunk\_len-1, & and beta + (j-1)*y\_chunk\_le
                                                                                                  (nghostz/2+1)+(k-1)*z_chunk_len:(nghostz/2+1)+k*z_chunk_len-1)
```

```
chunk(ntimes+1:ntimes+x_chunk_len,:ntimes,ntimes+1:ntimes+z_chunk_len) ...
1123,1128c1105
                                       chunk(ntimes+1:ntimes+x_chunk_len,&
                                               ntimes+y_chunk_len+1:,&
                                               ntimes+1:ntimes+z_chunk_len)&
                                               =yghost((nghost/2+1)+(i-1)&
                                               *x_chunk_len:(nghost/2+1)+i*x_chunk_len-1,ntimes+1:,&
                                               (\verb"nghostz/2+1") + (\verb"k-1") * \verb"z_chunk_len" : (\verb"nghostz/2+1") + \verb"k*z_chunk_len" - 1")
<
                                       chunk(ntimes+1:ntimes+x chunk len,ntimes+y chunk len+1:,ntimes+1:ntimes+z chunk len) ...
1130,1134c1107
                                       chunk(ntimes+1:ntimes+x chunk len.&
                                               ntimes+y_chunk_len+1:,ntimes+1:ntimes+z_chunk_len)&
                                               =cur((nghost/2+1)+(i-1)*x_chunk_len:(nghost/2+1)&
<
                                               +i*x_chunk_len-1,(nghost/2+1)+j*y_chunk_len:(nghost/2+1)+j*y_chunk_len+ntimes-1,&
                                               (\texttt{nghostz/2+1}) + (\texttt{k-1}) * \texttt{z\_chunk\_len:} (\texttt{nghostz/2+1}) + \texttt{k*z\_chunk\_len-1})
<
                                       chunk(ntimes+1:ntimes+x_chunk_len,ntimes+y_chunk_len+1:,ntimes+1:ntimes+z_chunk_len) ...
1140.1143c1113
                                       chunk(ntimes+1:ntimes+x chunk len.&
                                         ntimes+1:ntimes+y_chunk_len,:ntimes)&
                                         =zghost((nghost/2+1)+(i-1)*x_chunk_len:(nghost/2+1)+i*x_chunk_len-1,&
                                         (nghost/2+1)+(j-1)*y\_chunk\_len:(nghost/2+1)+j*y\_chunk\_len-1,:ntimes)
<
                                       chunk(ntimes+1:ntimes+x_chunk_len,ntimes+1:ntimes+y_chunk_len,:ntimes) ...
1145,1148c1115
                                       chunk(ntimes+1:ntimes+x_chunk_len,ntimes+1:ntimes+y_chunk_len,:ntimes)&
                                         (nghost/2+1)+(j-1)*y\_chunk\_len:(nghost/2+1)+j*y\_chunk\_len-1,\&
<
                                         (nghostz/2+1) + (k-1)*z\_chunk\_len-ntimes: (nghostz/2+1) + (k-1)*z\_chunk\_len-1)
                                       chunk(ntimes+1:ntimes+x_chunk_len,ntimes+1:ntimes+y_chunk_len,:ntimes) ...
1153,1155c1120
                                       =zghost((nghost/2+1)+(i-1)*x_chunk_len:(nghost/2+1)+i*x_chunk_len-1,&
<
                                         (nghost/2+1)+(j-1)*y_chunk_len:(nghost/2+1)+j*y_chunk_len-1,ntimes+1:)
                                       chunk(ntimes+1:ntimes+x_chunk_len,ntimes+1:ntimes+y_chunk_len,ntimes+z_chunk_len+1:) ...
1157,1160c1122
                                       chunk(ntimes+1:ntimes+x_chunk_len,ntimes+1:ntimes+y_chunk_len,ntimes+z_chunk_len+1:)&
                                         =cur((nghost/2+1)+(i-1)*x_chunk_len:(nghost/2+1)+i*x_chunk_len-1,&
<
                                         (nghost/2+1)+(j-1)*y\_chunk\_len:(nghost/2+1)+j*y\_chunk\_len-1,&
                                         (nghostz/2+1)+k*z_chunk_len:(nghostz/2+1)+k*z_chunk_len+ntimes-1)
                                       chunk(ntimes+1:ntimes+x_chunk_len,ntimes+1:ntimes+y_chunk_len,ntimes+z_chunk_len+1:) ...
1165,1168c1127
                               chunk(ntimes+1:ntimes+x_chunk_len,ntimes+1:ntimes+y_chunk_len,ntimes+1:ntimes+z_chunk_len)&
                                 =cur((nghost/2+1)+(i-1)*x_chunk_len:(nghost/2+1)+i*x_chunk_len-1,&
                                 (nghost/2+1)+(j-1)*y\_chunk\_len:(nghost/2+1)+j*y\_chunk\_len-1,&
                                 (nghostz/2+1)+(k-1)*z_chunk_len:(nghostz/2+1)+k*z_chunk_len-1)
                               chunk(ntimes+1:ntimes+x_chunk_len,ntimes+1:ntimes+y_chunk_len,ntimes+1:ntimes+z_chunk_len) ...
1171,1172c1130
                               call chunk_filter_x(chunk,2,ntimes+x_chunk_len+ntimes-1,&
                                                     1, ntimes+y_chunk_len+ntimes, 1, ntimes+z_chunk_len+ntimes)
___
                               call chunk_filter_x(chunk,2,ntimes+x_chunk_len+ntimes-1, ...
1175,1176c1133
                               call chunk filter y(chunk,1,ntimes+x chunk len+ntimes,2,&
                                                     ntimes+y_chunk_len+ntimes-1,1,ntimes+z_chunk_len+ntimes)
                               call chunk_filter_y(chunk,1,ntimes+x_chunk_len+ntimes,2, ...
1179.1180c1136
                               call chunk filter z(chunk,1,ntimes+x chunk len+ntimes,&
                                                     1,ntimes+y_chunk_len+ntimes,2,ntimes+z_chunk_len+ntimes-1)
<
                               call chunk_filter_z(chunk,1,ntimes+x_chunk_len+ntimes,1,ntimes+y_chunk_len+ntimes, ...
1184,1187c1140
                               (nghost/2+1)+(j-1)*y_chunk_len:(nghost/2+1)+j*y_chunk_len-1,&
                                      (nghostz/2+1)+(k-1)*z_chunk_len:(nghostz/2+1)+k*z_chunk_len-1)&
<
<
                                      =chunk(ntimes+1:ntimes+x_chunk_len,ntimes+1:ntimes+y_chunk_len,ntimes+1:ntimes+z_chunk_len)
                               temp(3+(i-1)*x\_chunk\_len:3+i*x\_chunk\_len-1,3+(j-1)*y\_chunk\_len:3+j*y\_chunk\_len-1,3+(k-1)* \dots
1192,1193c1145
       \verb|cur|((nghost/2+1):mx-(nghost/2+1),(nghost/2+1):my-(nghost/2+1):mz-(nghost/2+1))| \\
             =temp((nghost/2+1):mx-(nghost/2+1),(nghost/2+1):my-(nghost/2+1),(nghostz/2+1):mz-(nghostz/2+1))
<
       cur(3:mx-3,3:my-3,3:mz-3)=temp(3:mx-3,3:my-3,3:mz-3)
```

9 output.F90

9.1 save_spectrum_2d()

```
836,839c835,838
                mxmin=int((mx0-nghost)*.5)-1200+(nghost/2+1)
                mxmax=int((mx0-nghost)*.5)+400+(nghost/2+1)
                mymin=(nghost/2+1)
                mymax=my0-(nghost/2)
                mxmin=int((mx0-5)*.5)-1200+3
                mxmax=int((mx0-5)*.5)+400+3
                mymin=3
                mymax=my0-2
9.2 output_tot()
2648,2649c2647,2648
       kstart=(nghostz/2+1)
       kfinish=mz-(nghostz/2+1)
       kstart=3
       kfinish=mz-3
2669,2670c2668,2669
       jstart=nghost/2+1
       jfinish=my-(nghost/2+1)
<
       jstart=3
       ifinish=mv-3
2686,2687c2685,2686
      istart=nghost/2+1
       ifinish=mx-(nghost/2+1)
       istart=3
       ifinish=mx-3
3297c3296
       !goto 127
---
        goto 127
3546,3549c3545,3546
            if(varname.eq.'gammae') then
                temporary_vec(1:strd_lecs)=sqrt(1. &
                     +(p(lecs\_str\_ind)\%u**2+p(lecs\_str\_ind)\%v**2+p(lecs\_str\_ind)\%w**2))
<
---
             if(varname.eq.'gammae') temporary_vec(1:strd_lecs)=sqrt(1. &
               +(p(lecs\_str\_ind)\%u**2+p(lecs\_str\_ind)\%v**2+p(lecs\_str\_ind)\%w**2))
9.3 output_hug()
4006,4007c4003,4004
       kstart=(nghostz/2+1)
       kfinish=mz-(nghostz/2+1)
       kstart=3
4011c4008
< 1110 if(modulo(kstart+(rank/sizey)*(mzall-nghostz)-1*0,istep) .eq. 0) goto 1120
> 1110 if(modulo(kstart+(rank/sizey)*(mzall-5)-1*0,istep) .eq. 0) goto 1120
< 1130 if(modulo(kfinish+(rank/sizey)*(mzall-nghostz)-1*0,istep) .eq. 0) goto 1140
> 1130 if(modulo(kfinish+(rank/sizey)*(mzall-5)-1*0,istep) .eq. 0) goto 1140
4028,4029c4025,4026
      jstart=(nghost/2+1)
       jfinish=my-(nghost/2+1)
       istart=3
       jfinish=my-3
4033c4030
< 1210 if(modulo(jstart+modulo(rank,sizey)*(myall-nghost)-1*0,istep) .eq. 0) goto 1220
> 1210 if(modulo(jstart+modulo(rank,sizey)*(myall-5)-1*0,istep) .eq. 0) goto 1220
4038c4035
< 1230 if(modulo(jfinish+modulo(rank,sizey)*(myall-nghost)-1*0,istep) .eq. 0) goto 1240
> 1230 if(modulo(jfinish+modulo(rank,sizey)*(myall-5)-1*0,istep) .eq. 0) goto 1240
```

10 tristanmainloop.F90

Definitely keep $\mathtt{outcorner} = 1$, to avoid a numerical artifact. Without this, when partitioning the domain with \mathtt{sizex} and \mathtt{sizey} , particles in corner cells can be removed from the simulation. With only one call of $\mathtt{exchange_current}$ and $\mathtt{inject_particles}$, corner particles still end up in a ghost cell; these particles are determined to have $\mathtt{in} = \mathtt{false}$, and are removed from the simulation; some wave features can continue propagating in place of the removed particle. Keeping $\mathtt{outcorner} = 1$ ensures that even the particles in corner cells eventually end up in physical cells.

10.1 mainloop()

Record output at the beginning of the loop:

```
108,110c103
<
call Diagnostics()
<
---
>
114,119c107,108
<
call pre_bc_b()
```

The call to bc_e1() is present before advance_Bhalfstep() in case the high order field advance is used (the call to bc_b1() is redundant, and probably safe to remove). bc_e1() is also called so that the mover_lord, mover_2ord, mover_3ord routines see the correct field values in ghost cells. Without this call, a particle in a ghost cell would 'see' a zero field, only because fields had not been copied from the other side of the domain into the ghost cells. This leads to large error in the field interpolation, for particles whose stencils overlap with ghost cells.

```
<! print *, "advance b half" !hack
< call bc_b1()!USER
< call bc_e1()!USER
< call advance_Bhalfstep()
---

! Advance the Magnetic field half time step
print *, "prebc" !hack
120a110,113
> call pre_bc_b()
>! print *, "advance b half" !hack
> call advance_Bhalfstep()
```

bc_b1() is called after the field advance so that the mover_lord, mover_2ord, mover_3ord routines see correct field values in ghost cells.

These calls the bc_b1, bc_e1 are leftover from testing. Should be safe to remove.

Ghost cell modifications are untested with conduct_bc().

11 user_weibel.F90

12 Unmodified routines

- aux.F90
- communications.F90

Use of dynamic_domain will require updates to work with the ghost cell modifications (but we are willing to do it).

- dynamic_domain.F90
- fparser.F90
- globaldata.F90
- initialize.F90
- inputparserf.F90
- mpidummy.F90
- overload.F90
- restart.F90
- tristan.F90
- selectprt.F90
- systemf.F90

References

[1] Esirkepov, T. Z., 2001, Computer Physics Communications, 185, 708.