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! Skeleton 2-1/2D Electromagnetic GPU PIC code
! written by Viktor K. Decyk, UCLA
  program gpupic2
    use gpupush2
    use gpulib2
    use gpufft2
    implicit none
    integer, parameter :: indx = 9, indy = 9
    integer, parameter :: npx = 3072, npy = 3072
    integer, parameter :: ndim = 3
    real, parameter :: tend = 10.0, dt = 0.04, qme = -1.0
    real, parameter :: vtx = 1.0, vty = 1.0, vx0 = 0.0, vy0 = 0.0
    real, parameter :: vtz = 1.0, vz0 = 0.0
    real :: ax = .912871, ay = .912871, ci = 0.1
! idimp = dimension of phase space = 5
! relativity = (no,yes) = (0,1) = relativity is used
    integer :: idimp = 5, ipbc = 1, relativity = 1
    real :: wke = 0.0, we = 0.0, wf = 0.0, wm = 0.0, wt = 0.0
! sorting tiles
    integer :: mx = 16, my = 16
! fraction of extra particles needed for particle management
    real :: xtras = 0.2
! declare scalars for standard code
    integer :: np, nx, ny, nxh, nyh, nxh1, nxe, nye, nxeh, nxyh, nxhy
    integer :: mx1, my1, mxy1, ntime, nloop, isign
    real :: qbme, affp, dth
    real, dimension(1) :: sum
!
! declare scalars for GPU code
    integer :: nblock = 128
! nscache = (0,1,2) = (no,small,big) cache size
    integer :: nscache = 1
    integer :: mmcc, nppmx, nppmx0, ntmax, npbm
    integer :: nxhd
    integer, dimension(1) :: irc
!
! declare arrays for standard code
    real, dimension(:,:), pointer :: part
    complex, dimension(:,:), pointer :: ffct
    integer, dimension(:), pointer :: mixup
    complex, dimension(:), pointer :: sct
!
! declare arrays for GPU code
    integer, dimension(2) :: g_qe = 0.0
    integer, dimension(2) :: g_cue = 0.0, g_fxyz = 0.0, g_bxyz = 0.0
    integer, dimension(2) :: g_ffct = 0.0
    integer, dimension(2) :: g_mixup = 0.0, g_sct = 0.0
    integer, dimension(2) :: g_q = 0.0, g_cu = 0.0
    integer, dimension(2) :: g_qt = 0.0, g_cut = 0.0
    integer, dimension(2) :: g_fxyz = 0.0, g_hxyz = 0.0
    integer, dimension(2) :: g_fxyzt = 0.0, g_hxyzt = 0.0
    integer, dimension(2) :: g_exyzt = 0.0, g_bxyzt = 0.0
    integer, dimension(2) :: g_wke = 0.0, g_we = 0.0

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integer, dimension(2) :: g_wf = 0.0, g_wm = 0.0
integer, dimension(2) :: g_ppart = 0.0, g_ppbuff = 0.0
integer, dimension(2) :: g_kpic = 0.0
integer, dimension(2) :: g_ncl = 0.0, g_ihole = 0.0
integer, dimension(2) :: g_sum = 0.0
integer, dimension(2) :: g_irc = 0.0
complex, dimension(:,:,:), pointer :: qt
complex, dimension(:,:,:,:), pointer :: fxyzt
real, dimension(:,:,:,:), pointer :: ppart
integer, dimension(:), pointer :: kpic
!
! declare and initialize timing data
real :: time
integer, dimension(4) :: itime
double precision :: dtime
real :: tdpst = 0.0, tguard = 0.0, tffft = 0.0, tfield = 0.0
real :: tdjpost = 0.0, tpush = 0.0, tsort = 0.0
!
! initialize scalars for standard code
np = npx*npy; nx = 2**indx; ny = 2**indy; nxh = nx/2; nyh = ny/2
nxh1 = nxh + 1; nxe = nx + 2; nye = ny + 1; nxeh = nxe/2
nxyh = max(nx,ny)/2; nxhy = max(nxh,ny)
mx1 = (nx - 1)/mx + 1; my1 = (ny - 1)/my + 1; mxy1 = mx1*my1
nloop = tend/dt + .0001; ntime = 0
qbme = qme
affp = real(nx*ny)/real(np)
dth = 0.0
! set size for FFT arrays
nxhd = nxh1
!
! allocate and initialize data for standard code
allocate(part(idimp,np))
allocate(ffct(nyh,nxh))
allocate(mixup(nxhy),sct(nxyh))
allocate(kpic(mxy1))
allocate(qt(ny,nxh1),fxyzt(ny,ndim,nxh1))
!
! set up GPU
irc = 0
call gpu_setgbsize(nblock)
call init_cu(0,irc(1))
if (irc(1) /= 0) then
    write (*,*) 'CUDA initialization error!'
    stop
endif
! obtain compute capability
mmcc = getmmcc()
if (mmcc < 20) then
    write (*,*) 'compute capability 2.x or higher required'
    stop
endif
! set cache size
call gpu_set_cache_size(nscache)
!
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! allocate data for GPU code
call gpu_fallocate(g_qe,nxe*nye,irc(1))
call gpu_fallocate(g_cue,ndim*nxe*nye,irc(1))
call gpu_fallocate(g_fxyze,ndim*nxe*nye,irc(1))
call gpu_fallocate(g_bxyz,ndim*nxe*nye,irc(1))
call gpu_callocate(g_ffct,nyh*nxh,irc(1))
call gpu_iallocate(g_mixup,nxhy,irc(1))
call gpu_callocate(g_sct,nxyh,irc(1))
call gpu_callocate(g_q,nxhd*ny,irc(1))
call gpu_callocate(g_cu,nxhd*ndim*ny,irc(1))
call gpu_callocate(g_qt,ny*nxh1,irc(1))
call gpu_callocate(g_cut,ny*ndim*nxh1,irc(1))
call gpu_callocate(g_fxyz,nxhd*ndim*ny,irc(1))
call gpu_callocate(g_hxyz,nxhd*ndim*ny,irc(1))
call gpu_callocate(g_fxyzt,ny*ndim*nxh1,irc(1))
call gpu_callocate(g_hxyzt,ny*ndim*nxh1,irc(1))
call gpu_callocate(g_exyzt,ny*ndim*nxh1,irc(1))
call gpu_callocate(g_bxyzt,ny*ndim*nxh1,irc(1))
call gpu_fallocate(g_wke,mxy1,irc(1))
call gpu_fallocate(g_we,nxh1,irc(1))
call gpu_fallocate(g_wf,nxh1,irc(1))
call gpu_fallocate(g_wm,nxh1,irc(1))
call gpu_fallocate(g_sum,1,irc(1))
if (irc(1) /= 0) then
    write (*,*) 'GPU allocate error!'
    stop
endif

!
! prepare fft tables
call WFFT2RINIT(mixup,sct,indx,indy,nxhy,nxyh)
! prepare NVIDIA ffts
call gpufft2rrcuinit(nx,ny,ndim)
call gpufft2cuinit(nx,ny,ndim)
! calculate form factors
isign = 0
call POIS23T(qt,fxyzt,isign,ffct,ax,ay,affp,we,nx,ny,nxh1,ny,nxh, &
&nyh)
! copy in solver arrays to GPU
call gpu_icopyin(mixup,g_mixup,nxhy)
call gpu_ccopyin(sct,g_sct,nxyh)
call gpu_ccopyin(ffct,g_ffct,nyh*nxh)
! initialize electrons
call DISTR2H(part,vtx,vty,vtz,vx0,vy0,vz0,np,ny,idimp,np,nx,ny, &
&ipbc)
!
! initialize transverse electromagnetic fields
call gpu_zcmem(g_exyzt,ny*ndim*nxh1)
call gpu_zcmem(g_bxyzt,ny*ndim*nxh1)
!
! find number of particles in each of mx, my tiles: updates kpic, nppmx
call DBLKP2L(part,kpic,nppmx,idimp,np,mx,my,mx1,mxy1,irc)
if (irc(1) /= 0) then
    write (*,*) 'DBLKP2L error, irc=', irc
    stop

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        endif
! allocate vector particle data
    nppmx0 = (1.0 + xtras)*nppmx
    ntmax = 0.5*xtras*nppmx
    npbmx = 0.5*xtras*nppmx
! align data to warp size
    nppmx0 = 32*((nppmx0 - 1)/32 + 1)
    ntmax = 32*(ntmax/32 + 1)
    npbmx = 32*((npbmx - 1)/32 + 1)
    call gpu_fallocate(g_ppart,nppmx0*idimp*mxy1,irc(1))
    call gpu_fallocate(g_ppbuff,npbmx*idimp*mxy1,irc(1))
    call gpu_iallocate(g_kpic,mxy1,irc(1))
    call gpu_iallocate(g_ncl,8*mxy1,irc(1))
    call gpu_iallocate(g_ihole,2*(ntmax+1)*mxy1,irc(1))
    call gpu_iallocate(g irc,1,irc(1))
    if (irc(1) /= 0) then
        write (*,*) 'GPU allocate error!'
        stop
    endif
    allocate(ppart(nppmx0,idimp,mxy1))
!
! copy ordered particle data for GPU code: updates ppart and kpic
    call PPMOVIN2LT(part,ppart,kpic,nppmx0,idimp,np,mx,my,mx1,mxy1,irc&
    &)
    if (irc(1) /= 0) then
        write (*,*) 'PPMOVIN2LT overflow error, irc=', irc
        stop
    endif
! sanity check
    call PPCHECK2LT(ppart,kpic,idimp,nppmx0,nx,ny,mx,my,mx1,my1,irc)
    if (irc(1) /= 0) then
        write (*,*) 'PPCHECK2LT error: irc=', irc
        stop
    endif
! copy to GPU
    call gpu_icopyin(irc,g irc,1)
    call gpu_fcopyin(ppart,g ppart,nppmx0*idimp*mxy1)
    call gpu_icopyin(kpic,g kpic,mxy1)
!
    if (dt > 0.45*ci) then
        write (*,*) 'Warning: Courant condition may be exceeded!'
    endif
!
! * * * start main iteration loop * * *
!
500 if (nloop <= ntime) go to 2000
!     write (*,*) 'ntime = ', ntime
!
! deposit current with GPU code:
    call dtimer(dtime,itime,-1)
    call gpu_zfmem(g_cue,ndim*nxe*nye)
    if (relativity==1) then
! updates g_ppart, g_cue
        call cgpu2rjppost2l(g_ppart,g_cue,g_kpic,qme,dth,ci,nppmx0,      &

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    &idimp,nx,ny,mx,my,nxe,nye,mx1,mxy1,ipbc)
! updates g_ppart, g_cue, g_ncl, g_ihole, g_irc
!     call cgpu2rjppostf2l(g_ppart,g_cue,g_kpic,g_ncl,g_ihole,qme,dth&
!     &,ci,nppmx0,idimp,nx,ny,mx,my,nxe,nye,mx1,mxy1,ntmax,g_irc)
!         else
! updates g_ppart, g_cue
    call cgpu2jppost2l(g_ppart,g_cue,g_kpic,qme,dth,nppmx0,idimp,nx&
    &,ny,mx,my,nxe,nye,mx1,mxy1,ipbc)
! updates g_ppart, g_cue, g_ncl, g_ihole, g_irc
!     call cgpu2jppostf2l(g_ppart,g_cue,g_kpic,g_ncl,g_ihole,qme,dth,&
!     &nppmx0,idimp,nx,ny,mx,my,nxe,nye,mx1,mxy1,ntmax,g_irc)
!         endif
    call dtimer(dtime,itime,1)
    time = real(dtime)
    tdjpost = tdjpost + time
!
! reorder particles by tile with GPU code:
    call dtimer(dtime,itime,-1)
! updates g_ppart, g_ppbuff, g_kpic, g_ncl, g_ihole, and g_irc
    call cgpuppord2l(g_ppart,g_ppbuff,g_kpic,g_ncl,g_ihole,idimp,      &
    &nppmx0,nx,ny,mx,my,mx1,my1,npbmx,ntmax,g_irc)
! updates g_ppart, g_ppbuff, g_kpic, g_ncl, and g_irc
!     call cgpuppordf2l(g_ppart,g_ppbuff,g_kpic,g_ncl,g_ihole,idimp,      &
!     &nppmx0,mx1,my1,npbmx,ntmax,g_irc)
    call dtimer(dtime,itime,1)
    time = real(dtime)
    tsort = tsort + time
!
! deposit charge with GPU code: updates g_qe
    call dtimer(dtime,itime,-1)
    call gpu_zfmem(g_qe,nxe*nye)
    call cgpu2ppost2l(g_ppart,g_qe,g_kpic,qme,nppmx0,idimp,mx,my,nxe, &
    &nye,mx1,mxy1)
    call dtimer(dtime,itime,1)
    time = real(dtime)
    tdpst = tdpst + time
!
! add and copy guard cells with GPU code: updates g_q and g_cu
    call dtimer(dtime,itime,-1)
    call cgpucacguard2l(g_cu,g_cue,nx,ny,nxe,nye,nxhd,ny)
    call cgpucaguard2l(g_q,g_qe,nx,ny,nxe,nye,nxhd,ny)
    call dtimer(dtime,itime,1)
    time = real(dtime)
    tguard = tguard + time
!
! transform charge to fourier space with GPU code: updates g_q, g_qt
    call dtimer(dtime,itime,-1)
    isign = -1
    call cgpuffft2rcs(g_q,g_qt,isign,g_mixup,g_sct,indx,indy,nxhd,ny, &
    &nxhy,nxyh)
! NVIDIA fft
!     call gpufft2rrcu(g_q,g_qt,isign,indx,indy,nxhd,ny)
    call dtimer(dtime,itime,1)
    time = real(dtime)

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tfft = tfft + time
!
! transform current to fourier space with GPU code: updates g_cu, g_cut
    call dtimer(dtime,itime,-1)
    isign = -1
    call cgpuwfft2rcsn(g_cu,g_cut,isign,g_mixup,g_sct,indx,indy,ndim, &
&nxhd,ny,nxhy,nxyh)
! NVIDIA fft
    call gpufft2rrcun(g_cu,g_cut,isign,indx,indy,ndim,nxhd,ny)
    call dtimer(dtime,itime,1)
    time = real(dtime)
    tfft = tfft + time
!
! take transverse part of current with GPU code: updates g_cut
    call dtimer(dtime,itime,-1)
    call cgpucuperp2t(g_cut,nx,ny,nxhd,ny)
    call dtimer(dtime,itime,1)
    time = real(dtime)
    tfield = tfield + time
!
! calculate electromagnetic fields in fourier space with GPU code:
! updates g_exyzt, g_bxyzt, g_wf, g_wm
    call dtimer(dtime,itime,-1)
    if (ntime==0) then
        call cgpuibpois23t(g_cut,g_bxyzt,g_ffct,ci,g_wm,nx,ny,nxh1,ny, &
&nxh,nyh)
        call gpu_zfmem(g_wf,nxh1)
        dth = 0.5*dt
    else
        call cgpumaxwel2t(g_exyzt,g_bxyzt,g_cut,g_ffct,ci,dt,g_wf,g_wm, &
&nx,ny,nxh1,ny,nxh,nyh)
        endif
    call dtimer(dtime,itime,1)
    time = real(dtime)
    tfield = tfield + time
!
! calculate force/charge in fourier space with GPU code:
! updates g_fxyzt, g_we
    call dtimer(dtime,itime,-1)
    call cgpupois23t(g_qt,g_fxyzt,g_ffct,g_we,nx,ny,nxh1,ny,nxh,nyh)
    call dtimer(dtime,itime,1)
    time = real(dtime)
    tfield = tfield + time
!
! add longitudinal and transverse electric fields with with GPU code:
! updates g_fxyzt
    call dtimer(dtime,itime,-1)
    isign = 1
    call cgpuemfield2t(g_fxyzt,g_exyzt,g_ffct,isign,nx,ny,nxh1,ny,nxh, &
&nyh)
! copy magnetic field with GPU code: updates g_hxyzt
    isign = -1
    call cgpuemfield2t(g_hxyzt,g_bxyzt,g_ffct,isign,nx,ny,nxh1,ny,nxh, &
&nyh)

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    call dtimer(dtime,itime,1)
    time = real(dtime)
    tfield = tfield + time

!
! transform electric force to real space with GPU code:
! updates g_fxyzt, g_fxyz
    call dtimer(dtime,itime,-1)
    isign = 1
    call cgpuwfft2rcsn(g_fxyz,g_fxyzt,isign,g_mixup,g_sct,indx,indy, &
&ndim,nxhd,ny,nxhy,nxyh)

! NVIDIA fft
!     call gpufft2rrcun(g_fxyz,g_fxyzt,isign,indx,indy,ndim,nxhd,ny)
!     call dtimer(dtime,itime,1)
!     time = real(dtime)
!     tfft = tfft + time

!
! transform magnetic force to real space with GPU code:
! updates g_hxyzt, g_hxyz
    call dtimer(dtime,itime,-1)
    isign = 1
    call cgpuwfft2rcsn(g_hxyz,g_hxyzt,isign,g_mixup,g_sct,indx,indy, &
&ndim,nxhd,ny,nxhy,nxyh)

! NVIDIA fft
!     call gpufft2rrcun(g_hxyz,g_hxyzt,isign,indx,indy,ndim,nxhd,ny)
!     call dtimer(dtime,itime,1)
!     time = real(dtime)
!     tfft = tfft + time

!
! copy guard cells with GPU code: updates g_fxyz, g_bxyz
    call dtimer(dtime,itime,-1)
    call cgpucbguard2l(g_fxyz,g_fxyz,nx,ny,nxe,nye,nxhd,ny)
    call cgpucbguard2l(g_hxyz,g_bxyz,nx,ny,nxe,nye,nxhd,ny)
    call dtimer(dtime,itime,1)
    time = real(dtime)
    tguard = tguard + time

!
! push particles with GPU code:
    call dtimer(dtime,itime,-1)
    if (relativity==1) then
! updates g_ppart, g_wke
        call cgpurbppush23l(g_ppart,g_fxyz,g_bxyz,g_kpic,qbme,dt,dth, &
        &ci,g_wke,idimp,nppmx0,nx,ny,mx,my,nxe,nye,mx1,mxy1,ipbc)
! updates g_ppart, g_ncl, g_ihole, g_wke, g_irc
        call cgpurbppushf23l(g_ppart,g_fxyz,g_bxyz,g_kpic,g_ncl, &
        &g_ihole,qbme,dt,dth,ci,g_wke,idimp,nppmx0,nx,ny,mx,my,nxe,nye,mx1, &
        &mxy1,ntmax,g_irc)
        else
! updates g_ppart, g_wke
        call cgpubbppush23l(g_ppart,g_fxyz,g_bxyz,g_kpic,qbme,dt,dth, &
        &g_wke,idimp,nppmx0,nx,ny,mx,my,nxe,nye,mx1,mxy1,ipbc)
! updates g_ppart, g_ncl, g_ihole, g_wke, g_irc
        call cgpubbppushf23l(g_ppart,g_fxyz,g_bxyz,g_kpic,g_ncl, &
        &g_ihole,qbme,dt,dth,g_wke,idimp,nppmx0,nx,ny,mx,my,nxe,nye,mx1, &
        &mxy1,ntmax,g_irc)

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        endif
        call dtimer(dtime,itime,1)
        time = real(dtime)
        tpush = tpush + time
!
! reorder particles by tile with GPU code:
        call dtimer(dtime,itime,-1)
! updates g_ppart, g_ppbuff, g_kpic, g_ncl, g_ihole, and g_irc
        call cgpuppor21(g_ppart,g_ppbuff,g_kpic,g_ncl,g_ihole,idimp,      &
                      &nppmx0,nx,ny,mx,my,mx1,my1,npbmx,ntmax,g_irc)
! updates g_ppart, g_ppbuff, g_kpic, g_ncl, and g_irc
!     call cgpuppor21(g_ppart,g_ppbuff,g_kpic,g_ncl,g_ihole,idimp,      &
!     &nppmx0,mx1,my1,npbmx,ntmax,g_irc)
        call dtimer(dtime,itime,1)
        time = real(dtime)
        tsort = tsort + time
!
! sanity check
        call gpu_icopyout(irc,g_irc,1)
        if (irc(1) /= 0) then
            write (*,*) 'deposit/push/reorder error: ntmax, irc=',ntmax,irc
            stop
        endif
!
! energy diagnostic
        if (ntime==0) then
            call gpu_zfmem(g_sum,1)
            call cgpusum2(g_we,g_sum,nxh1)
            call gpu_fcopyout(sum,g_sum,1); we = sum(1)
            call gpu_zfmem(g_sum,1)
            call cgpusum2(g_wf,g_sum,nxh1)
            call gpu_fcopyout(sum,g_sum,1); wf = sum(1)
            call gpu_zfmem(g_sum,1)
            call cgpusum2(g_wm,g_sum,nxh1)
            call gpu_fcopyout(sum,g_sum,1); wm = sum(1)
            call gpu_zfmem(g_sum,1)
            call cgpusum2(g_wke,g_sum,mxy1)
            call gpu_fcopyout(sum,g_sum,1); wke = sum(1)
            wt = we + wf + wm
            write (*,*) 'Initial Total Field, Kinetic and Total Energies:'
            write (*,'(3e14.7)') wt, wke, wke + wt
            write (*,*) 'Initial Electrostatic, Transverse Electric and Mag&
&netic Field Energies:'
            write (*,'(3e14.7)') we, wf, wm
        endif
        ntime = ntime + 1
        go to 500
500    continue
!
! * * * end main iteration loop * * *
!
        write (*,*) 'ntime = ', ntime
        write (*,*) 'relativity = ', relativity
! energy diagnostic

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call gpu_zfmem(g_sum,1)
call cgpusum2(g_we,g_sum,nxh1)
call gpu_fcopyout(sum,g_sum,1); we = sum(1)
call gpu_zfmem(g_sum,1)
call cgpusum2(g_wf,g_sum,nxh1)
call gpu_fcopyout(sum,g_sum,1); wf = sum(1)
call gpu_zfmem(g_sum,1)
call cgpusum2(g_wm,g_sum,nxh1)
call gpu_fcopyout(sum,g_sum,1); wm = sum(1)
call gpu_zfmem(g_sum,1)
call cgpusum2(g_wke,g_sum,mxy1)
call gpu_fcopyout(sum,g_sum,1); wke = sum(1)
wt = we + wf + wm
write (*,*) 'Final Total Field, Kinetic and Total Energies:'
write (*,'(3e14.7)') wt, wke, wke + wt
write (*,*) 'Final Electrostatic, Transverse Electric and Magnetic&
& Field Energies:'
write (*,'(3e14.7)') we, wf, wm
!
write (*,*)
write (*,*) 'deposit time = ', tdpost
write (*,*) 'current deposit time = ', tdjpost
tdpost = tdpost + tdjpost
write (*,*) 'total deposit time = ', tdpost
write (*,*) 'guard time = ', tguard
write (*,*) 'solver time = ', tfield
write (*,*) 'fft time = ', tfft
write (*,*) 'push time = ', tpush
write (*,*) 'sort time = ', tsort
tfield = tfield + tguard + tfft
write (*,*) 'total solver time = ', tfield
time = tdpost + tpush + tsort
write (*,*) 'total particle time = ', time
wt = time + tfield
write (*,*) 'total time = ', wt
write (*,*)

!
wt = 1.0e+09/(real(nloop)*real(np))
write (*,*) 'Push Time (nsec) = ', tpush*wt
write (*,*) 'Deposit Time (nsec) = ', tdpost*wt
write (*,*) 'Sort Time (nsec) = ', tsort*wt
write (*,*) 'Total Particle Time (nsec) = ', time*wt
write (*,*)

!
! close down NVIDIA fft
call gpufft2cudel()
call gpufft2rrcudel()
! deallocate memory on GPU
call gpu_deallocate(g_irc,irc(1))
call gpu_deallocate(g_ihole,irc(1))
call gpu_deallocate(g_ncl,irc(1))
call gpu_deallocate(g_kpic,irc(1))
call gpu_deallocate(g_sum,irc(1))
call gpu_deallocate(g_wm,irc(1))

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call gpu_deallocate(g_wf,irc(1))
call gpu_deallocate(g_we,irc(1))
call gpu_deallocate(g_wke,irc(1))
call gpu_deallocate(g_bxyzt,irc(1))
call gpu_deallocate(g_exyzt,irc(1))
call gpu_deallocate(g_hxyzt,irc(1))
call gpu_deallocate(g_fxyzt,irc(1))
call gpu_deallocate(g_hxyz,irc(1))
call gpu_deallocate(g_fxyz,irc(1))
call gpu_deallocate(g_cut,irc(1))
call gpu_deallocate(g_qt,irc(1))
call gpu_deallocate(g_cu,irc(1))
call gpu_deallocate(g_q,irc(1))
call gpu_deallocate(g_sct,irc(1))
call gpu_deallocate(g_mixup,irc(1))
call gpu_deallocate(g_ffct,irc(1))
call gpu_deallocate(g_ppbuff,irc(1))
call gpu_deallocate(g_ppart,irc(1))
call gpu_deallocate(g_bxyz,irc(1))
call gpu_deallocate(g_fxyz,irc(1))
call gpu_deallocate(g_cue,irc(1))
call gpu_deallocate(g_qe,irc(1))
! close down GPU
    call end_cu()
!
stop
end program
```