OpenMP® Offloading Support for VASP Using Cray Compiler

Presenter: Mahdieh Ghazimirsaeed

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AMD
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Contributors

- Leopold Grinberg
- Bill Brantley
- Michael Klemm
- Justin Chang
- Ossian OReily
- Paul Mullowney
- Asitav Mishra

Content

- **Introduction**
- Debugging and profiling OpenMP offloading code in VASP
- OpenMP Offloading Challenges in VASP
  - Concurrent support for different directive-based paradigms
  - Enable/disable offloading in different code paths
  - Interface OMP offloading with ROCM libraries
- Compiler related challenges
  - Pointer aliasing
  - Pointer mismatch in subroutine calls
  - Atomic update
  - Declare target
- Data management
- Summary

VASP (Vienna Ab Initio Simulation Package)

- A computer program for atomic scale materials modelling, e.g., electronic structure calculations and quantum-mechanical molecular dynamics
- Currently used by more than 1400 research groups in academia and industry worldwide
- Software license agreements with the University of Vienna
- ~550K lines of FORTRAN 90 code (some FORTRAN 77)

VASP support for directive-based and distributed programming

- Latest version: VASP.6.3.2 released in June 2022
- Supports MPI, OpenMP, and OpenACC
- Support for directive-based programming
  - OpenMP support for execution on the host
  - OpenACC support for execution on GPUs
- Working on adding support for OpenMP offloading to enable VASP execution on GPUs with OpenMP
  - Cray Compiler

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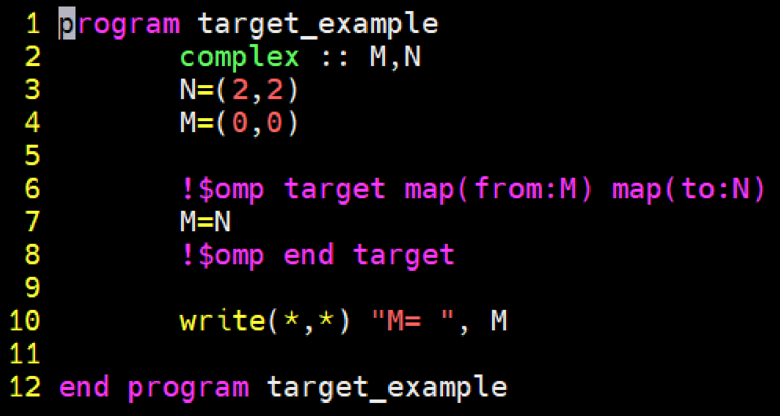
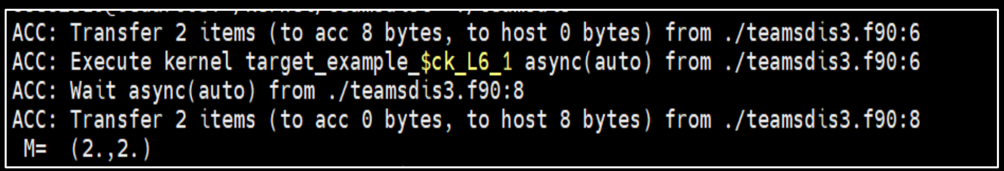
Debugging with Cray compiler: CRAY_ACC_DEBUG

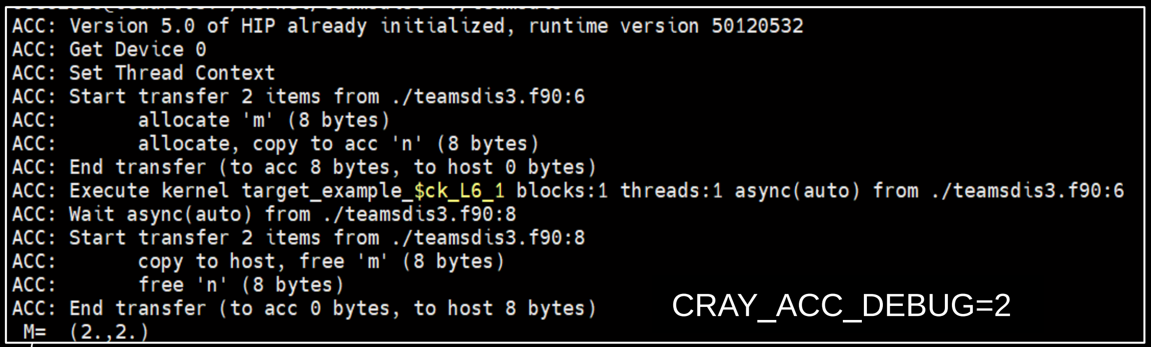


```fortran
program target_example
        complex :: M,N
        N=(2,2)
        M=(0,0)

        !$omp target map(from:M) map(to:N)
        M=N
        !$omp end target

        write(*,*) "M= ", M

end program target_example
```

CRAY_ACC_DEBUG=1

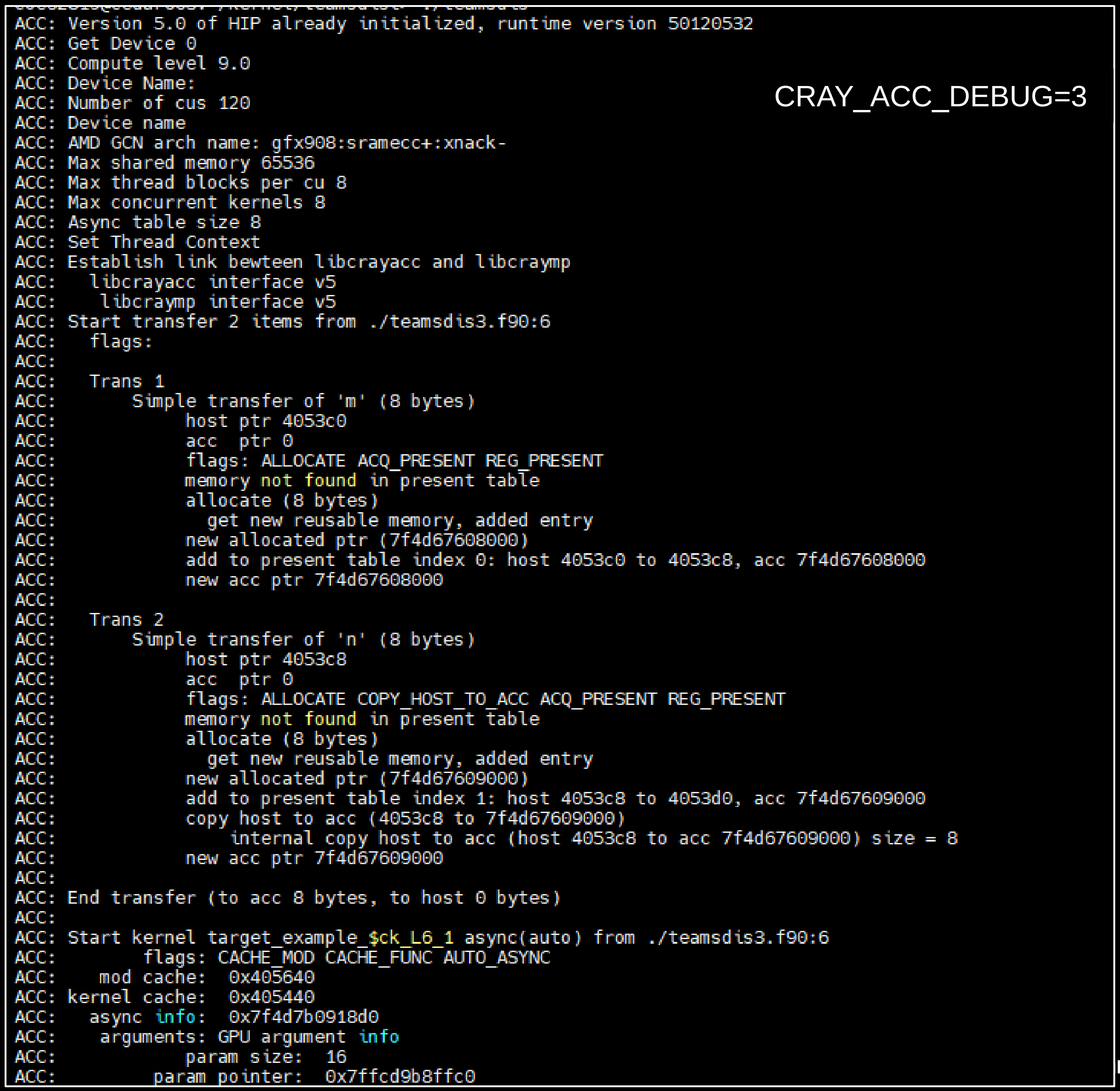


```
ACC: Transfer 2 items (to acc 8 bytes, to host 0 bytes) from ./teamsdis3.f90:6
ACC: Execute kernel target_example_$ck_L6_1 async(auto) from ./teamsdis3.f90:6
ACC: Wait async(auto) from ./teamsdis3.f90:8
ACC: Transfer 2 items (to acc 0 bytes, to host 8 bytes) from ./teamsdis3.f90:8
 M=  (2.,2.)
```



```
ACC: Version 5.0 of HIP already initialized, runtime version 50120532
ACC: Get Device 0
ACC: Set Thread Context
ACC: Start transfer 2 items from ./teamsdis3.f90:6
ACC:       allocate 'm' (8 bytes)
ACC:       allocate, copy to acc 'n' (8 bytes)
ACC: End transfer (to acc 8 bytes, to host 0 bytes)
ACC: Execute kernel target_example_$ck_L6_1 blocks:1 threads:1 async(auto) from ./teamsdis3.f90:6
ACC: Wait async(auto) from ./teamsdis3.f90:8
ACC: Start transfer 2 items from ./teamsdis3.f90:8
ACC:       copy to host, free 'm' (8 bytes)
ACC:       free 'n' (8 bytes)
ACC: End transfer (to acc 0 bytes, to host 8 bytes)
 M=  (2.,2.)
```

CRAY_ACC_DEBUG=2

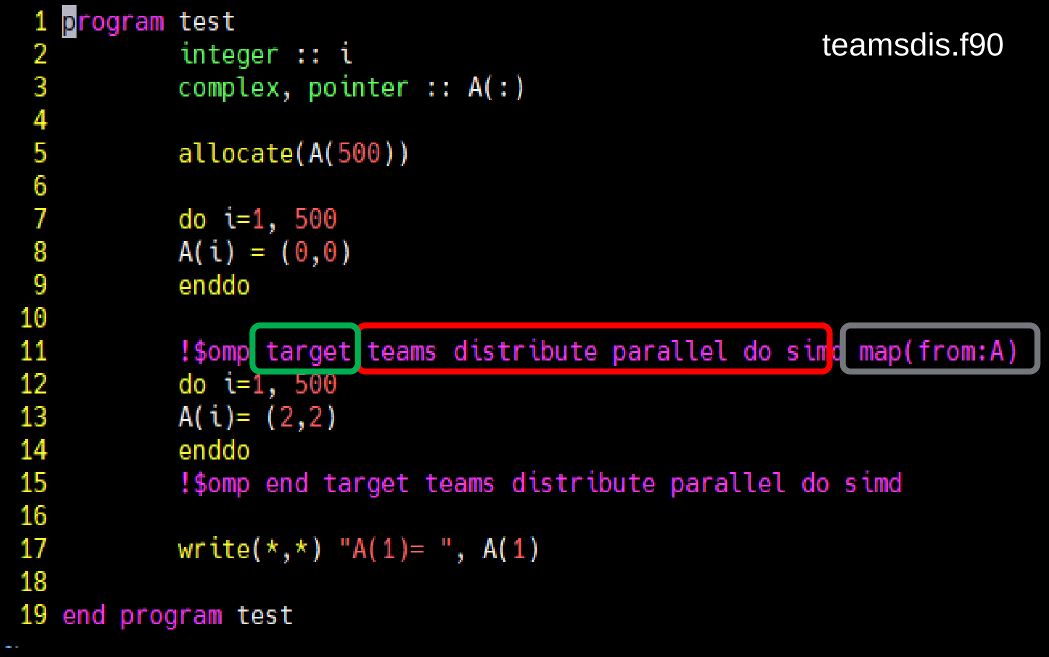


CRAY_ACC_DEBUG=3

```
ACC: Version 5.0 of HIP already initialized, runtime version 50120532
ACC: Get Device 0
ACC: Compute level 9.0
ACC: Device Name:
ACC: Number of cus 120
ACC: Device name
ACC: AMD GCN arch name: gfx908:sramecc+:xnack-
ACC: Max shared memory 65536
ACC: Max thread blocks per cu 8
ACC: Max concurrent kernels 8
ACC: Async table size 8
ACC: Set Thread Context
ACC: Establish link bewteen libcrayacc and libcraymp
ACC:   libcrayacc interface v5
ACC:    libcraymp interface v5
ACC: Start transfer 2 items from ./teamsdis3.f90:6
ACC:   flags:
ACC:
ACC:   Trans 1
ACC:       Simple transfer of 'm' (8 bytes)
ACC:            host ptr 4053c0
ACC:            acc  ptr 0
ACC:            flags: ALLOCATE ACQ_PRESENT REG_PRESENT
ACC:            memory not found in present table
ACC:            allocate (8 bytes)
ACC:              get new reusable memory, added entry
ACC:            new allocated ptr (7f4d67608000)
ACC:            add to present table index 0: host 4053c0 to 4053c8, acc 7f4d67608000
ACC:            new acc ptr 7f4d67608000
ACC:
ACC:   Trans 2
ACC:       Simple transfer of 'n' (8 bytes)
ACC:            host ptr 4053c8
ACC:            acc  ptr 0
ACC:            flags: ALLOCATE COPY_HOST_TO_ACC ACQ_PRESENT REG_PRESENT
ACC:            memory not found in present table
ACC:            allocate (8 bytes)
ACC:              get new reusable memory, added entry
ACC:            new allocated ptr (7f4d67609000)
ACC:            add to present table index 1: host 4053c8 to 4053d0, acc 7f4d67609000
ACC:            copy host to acc (4053c8 to 7f4d67609000)
ACC:                internal copy host to acc (host 4053c8 to acc 7f4d67609000) size = 8
ACC:            new acc ptr 7f4d67609000
ACC:
ACC: End transfer (to acc 8 bytes, to host 0 bytes)
ACC:
ACC: Start kernel target_example_$ck_L6_1 async(auto) from ./teamsdis3.f90:6
ACC:        flags: CACHE_MOD CACHE_FUNC AUTO_ASYNC
ACC:    mod cache:  0x405640
ACC: kernel cache:  0x405440
ACC:   async info:  0x7f4d7b0918d0
ACC:    arguments: GPU argument info
ACC:            param size:  16
ACC:         param pointer:  0x7ffcd9b8ffc0
```

Debugging with Cray compiler: –hlist=aimd

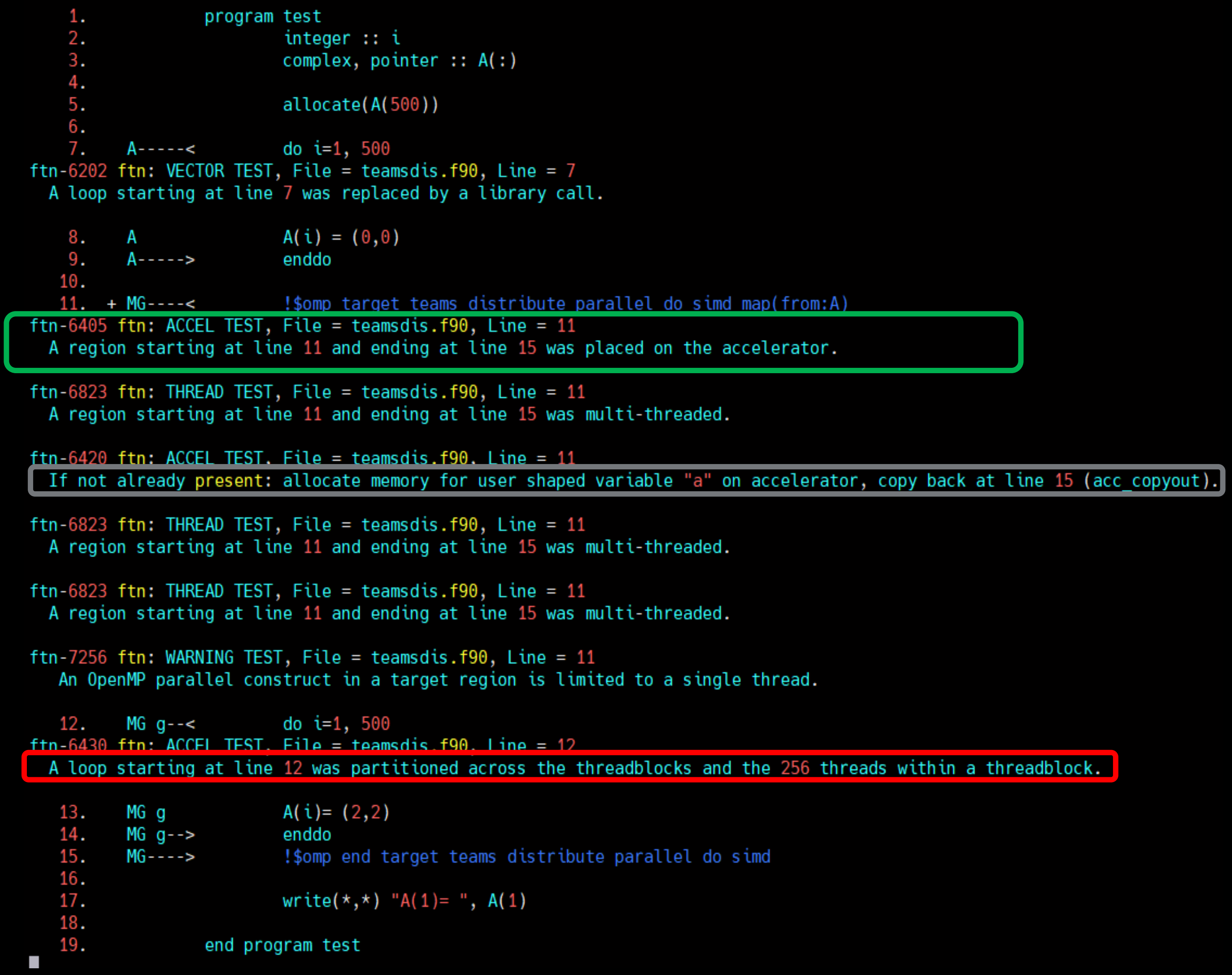
*.lst



teamsdis.f90

```
 1 program test
 2         integer :: i
 3         complex, pointer :: A(:)
 4
 5         allocate(A(500))
 6
 7         do i=1, 500
 8         A(i) = (0,0)
 9         enddo
10
11         !$omp target teams distribute parallel do simd map(from:A)
12         do i=1, 500
13         A(i)= (2,2)
14         enddo
15         !$omp end target teams distribute parallel do simd
16
17         write(*,*) "A(1)= ", A(1)
18
19 end program test
```

$ftn -hnoacc -homp -fopenmp -hlist=aimd -o ./teamsdis ./teamsdis.f90



```
    1.            program test
    2.                    integer :: i
    3.                    complex, pointer :: A(:)
    4.
    5.                    allocate(A(500))
    6.
    7.    A----<          do i=1, 500
ftn-6202 ftn: VECTOR TEST, File = teamsdis.f90, Line = 7
  A loop starting at line 7 was replaced by a library call.

    8.    A               A(i) = (0,0)
    9.    A---->          enddo
   10.
   11.  + MG----<         !$omp target teams distribute parallel do simd map(from:A)
ftn-6405 ftn: ACCEL TEST, File = teamsdis.f90, Line = 11
  A region starting at line 11 and ending at line 15 was placed on the accelerator.

ftn-6823 ftn: THREAD TEST, File = teamsdis.f90, Line = 11
  A region starting at line 11 and ending at line 15 was multi-threaded.

ftn-6420 ftn: ACCEL TEST, File = teamsdis.f90, Line = 11
  If not already present: allocate memory for user shaped variable "a" on accelerator, copy back at line 15 (acc_copyout).

ftn-6823 ftn: THREAD TEST, File = teamsdis.f90, Line = 11
  A region starting at line 11 and ending at line 15 was multi-threaded.

ftn-6823 ftn: THREAD TEST, File = teamsdis.f90, Line = 11
  A region starting at line 11 and ending at line 15 was multi-threaded.

ftn-7256 ftn: WARNING TEST, File = teamsdis.f90, Line = 11
   An OpenMP parallel construct in a target region is limited to a single thread.

   12.    MG g--<         do i=1, 500
ftn-6430 ftn: ACCEL TEST, File = teamsdis.f90, Line = 12
  A loop starting at line 12 was partitioned across the threadblocks and the 256 threads within a threadblock.

   13.    MG g            A(i)= (2,2)
   14.    MG g-->         enddo
   15.    MG---->         !$omp end target teams distribute parallel do simd
   16.
   17.                    write(*,*) "A(1)= ", A(1)
   18.
   19.            end program test
```

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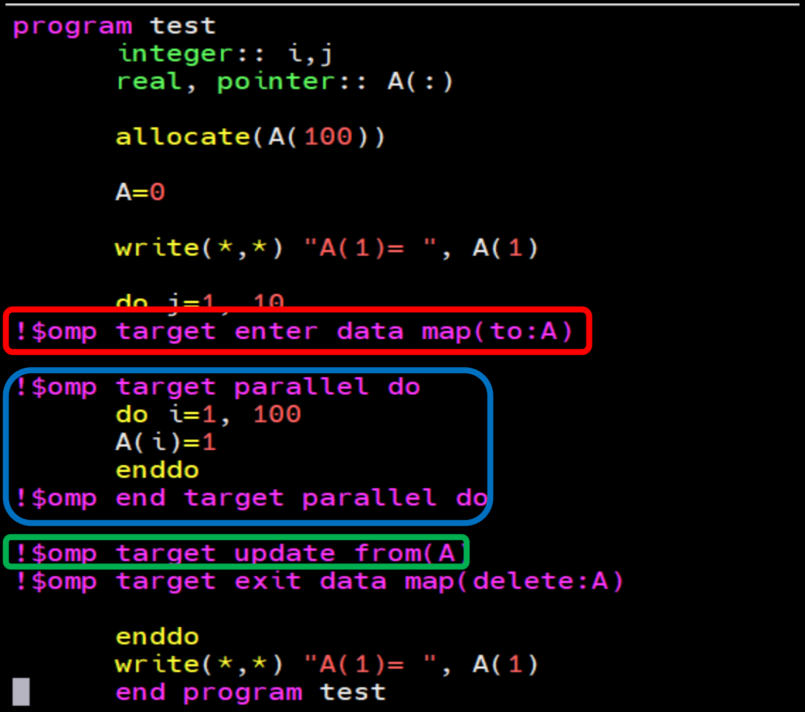
Profiling OpenMP® offloading code on AMD GPUs

- After compiling the code, run it with “rocprof --hip-trace”

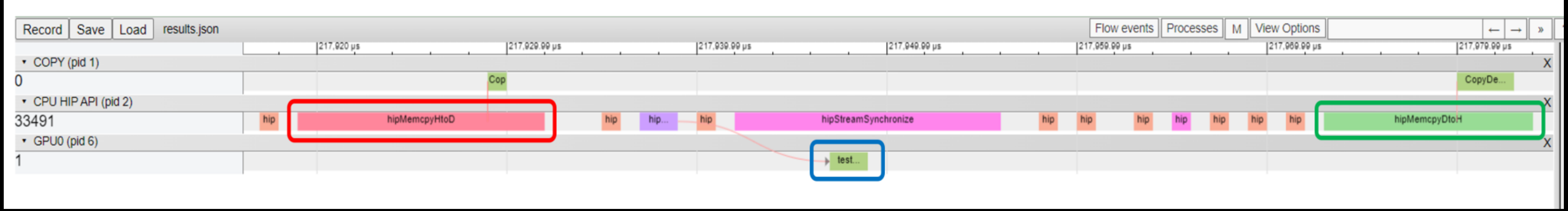
  $ftn -hnoacc -fopenmp -homp -o ./test ./test.f90

  $rocprof --hip-trace ./test

- Open the .json file in chrome://tracing/ or https://ui.perfetto.dev/

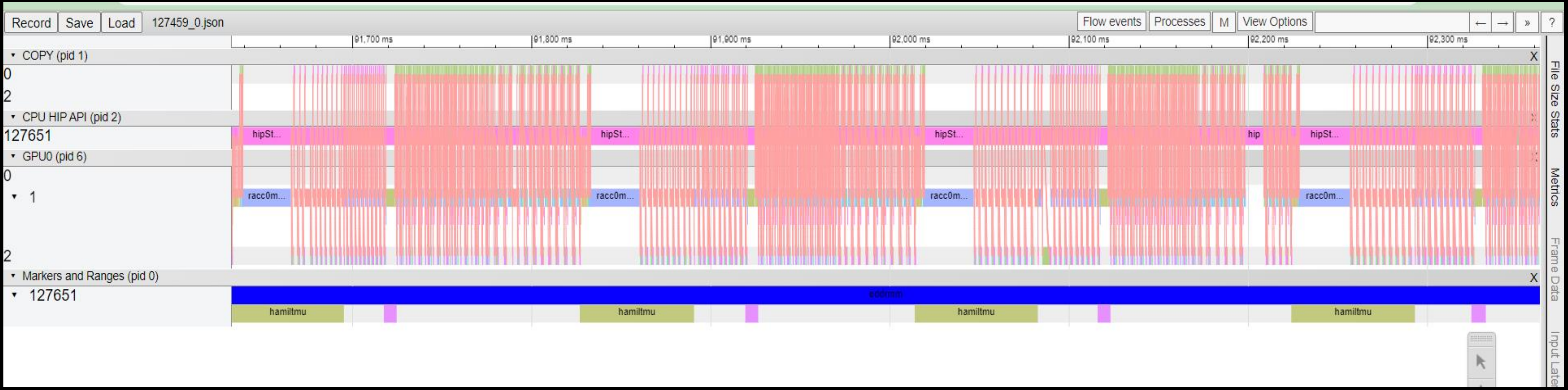


```
program test
      integer:: i,j
      real, pointer:: A(:)

      allocate(A(100))

      A=0

      write(*,*) "A(1)= ", A(1)

      do j=1, 10
!$omp target enter data map(to:A)

!$omp target parallel do
      do i=1, 100
      A(i)=1
      enddo
!$omp end target parallel do

!$omp target update from(A
!$omp target exit data map(delete:A)

      enddo
      write(*,*) "A(1)= ", A(1)
      end program test
```



An example of VASP trace on AMD GPUs

- Use markers to map trace with different sections of the code
  - add roctxRangePushA() and roctxRangePop()
  - Compile with “-lroctx64 –lroctracer64”
  - Run with “rocprof –hip-trace –roctx-trace”



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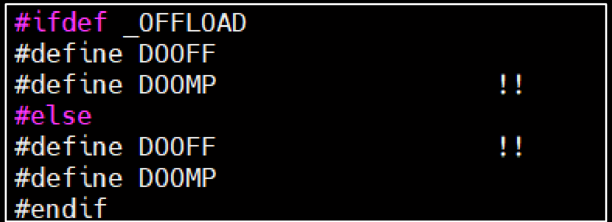
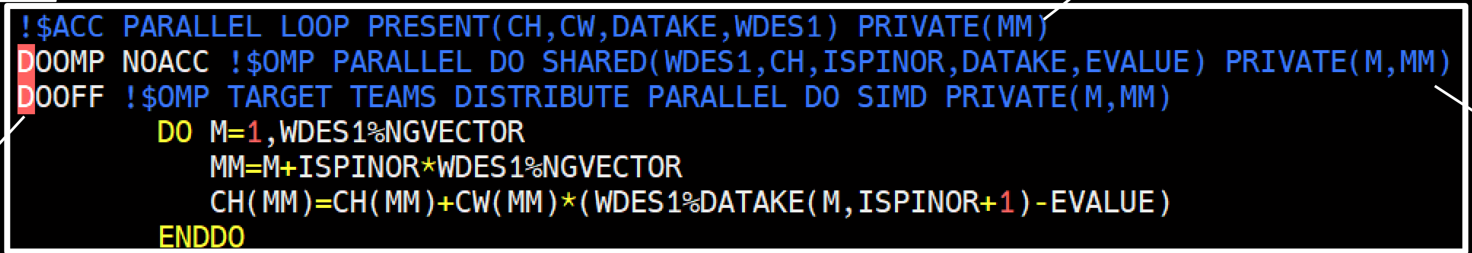
Supporting concurrent directive-based paradigms in VASP

- Switch between different directive-based paradigms without letting them impact on each other
- Take advantage of source preprocessing
  - Pros: switch between different directive-based paradigms
  - Cons: makes the code messy



```
#ifdef _OFFLOAD
#define DOOFF
#define DOOMP                  !!
#else
#define DOOFF                  !!
#define DOOMP
#endif
```

Used when VASP is compiled with OpenACC



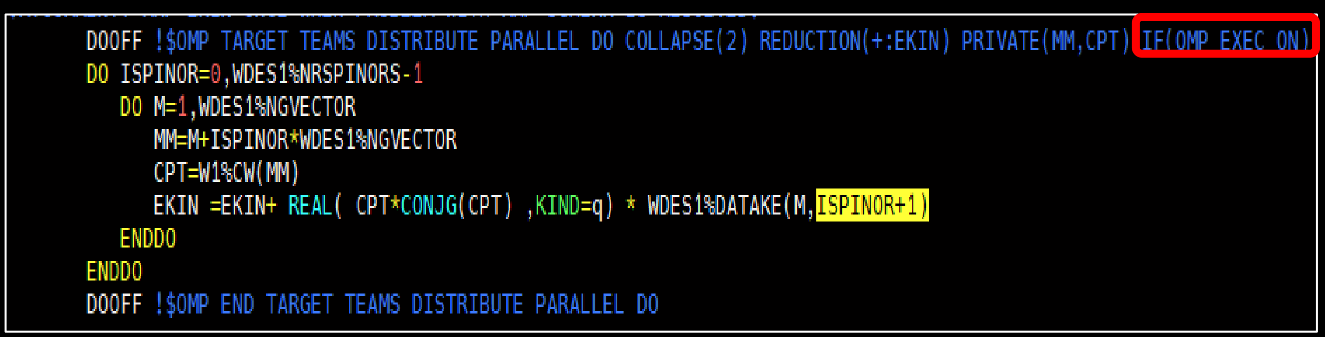
```
!$ACC PARALLEL LOOP PRESENT(CH,CW,DATAKE,WDES1) PRIVATE(MM)
DOOMP NOACC !$OMP PARALLEL DO SHARED(WDES1,CH,ISPINOR,DATAKE,EVALUE) PRIVATE(M,MM)
DOOFF !$OMP TARGET TEAMS DISTRIBUTE PARALLEL DO SIMD PRIVATE(M,MM)
        DO M=1,WDES1%NGVECTOR
           MM=M+ISPINOR*WDES1%NGVECTOR
           CH(MM)=CH(MM)+CW(MM)*(WDES1%DATAKE(M,ISPINOR+1)-EVALUE)
        ENDDO
```

Used when OpenMP offloading is enabled

Used when OpenMP (host) is enabled and OpenMP offloading/OpenACC is disabled

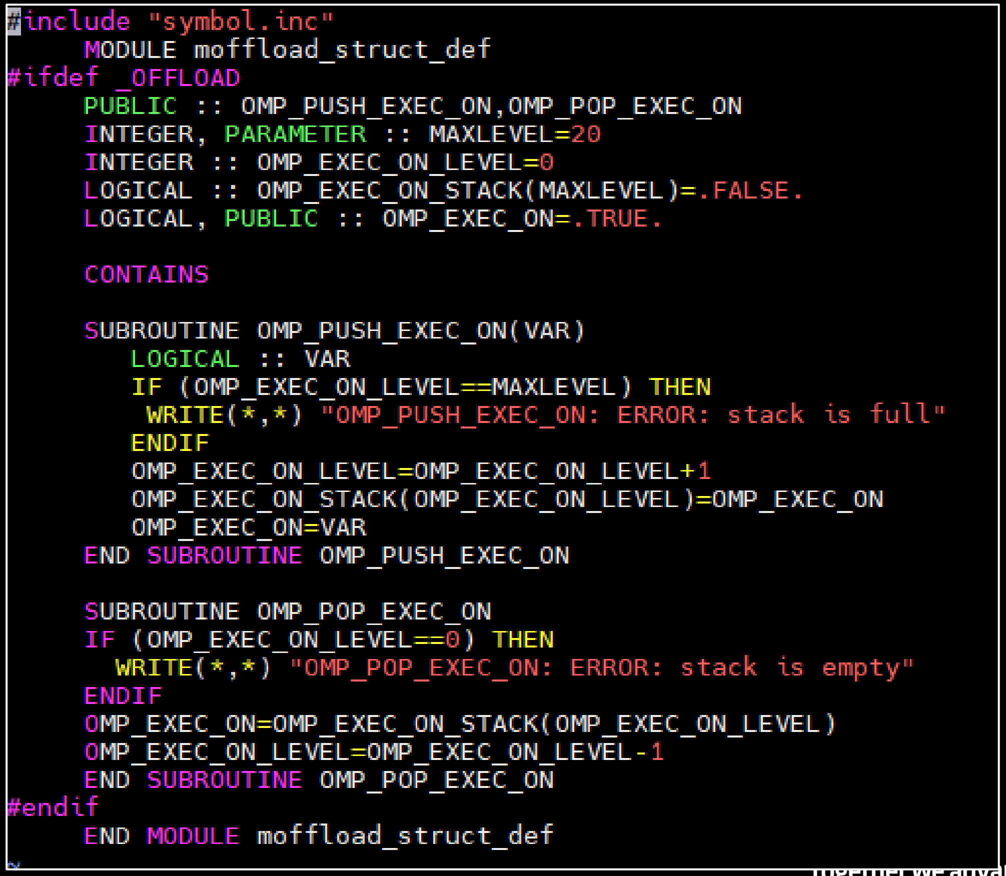
Enable/disable offloading in different code paths

- Many of the VASP subroutines are called from different code paths
  - How can we enable offloading for a subroutine in one path and disable offloading for others
    - It would be useful for code development and debugging



```
      DOOFF !$OMP TARGET TEAMS DISTRIBUTE PARALLEL DO COLLAPSE(2) REDUCTION(+:EKIN) PRIVATE(MM,CPT) IF(OMP_EXEC_ON)
      DO ISPINOR=0,WDES1%NRSPINORS-1
         DO M=1,WDES1%NGVECTOR
            MM=M+ISPINOR*WDES1%NGVECTOR
            CPT=W1%CW(MM)
            EKIN =EKIN+ REAL( CPT*CONJG(CPT) ,KIND=q) * WDES1%DATAKE(M,ISPINOR+1)
         ENDDO
      ENDDO
      DOOFF !$OMP END TARGET TEAMS DISTRIBUTE PARALLEL DO
```

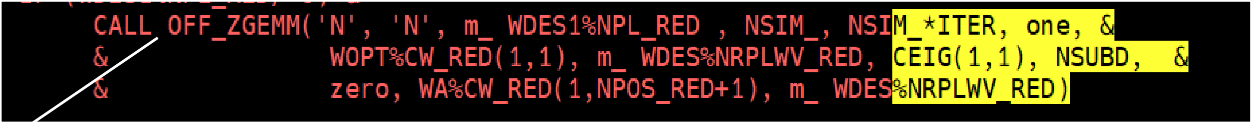
We can call OMP_PUSH_EXEC_ON(.TRUE.) or OMP_PUSH_EXEC_ON(.FALSE.) to enable or disable offloading in different code paths



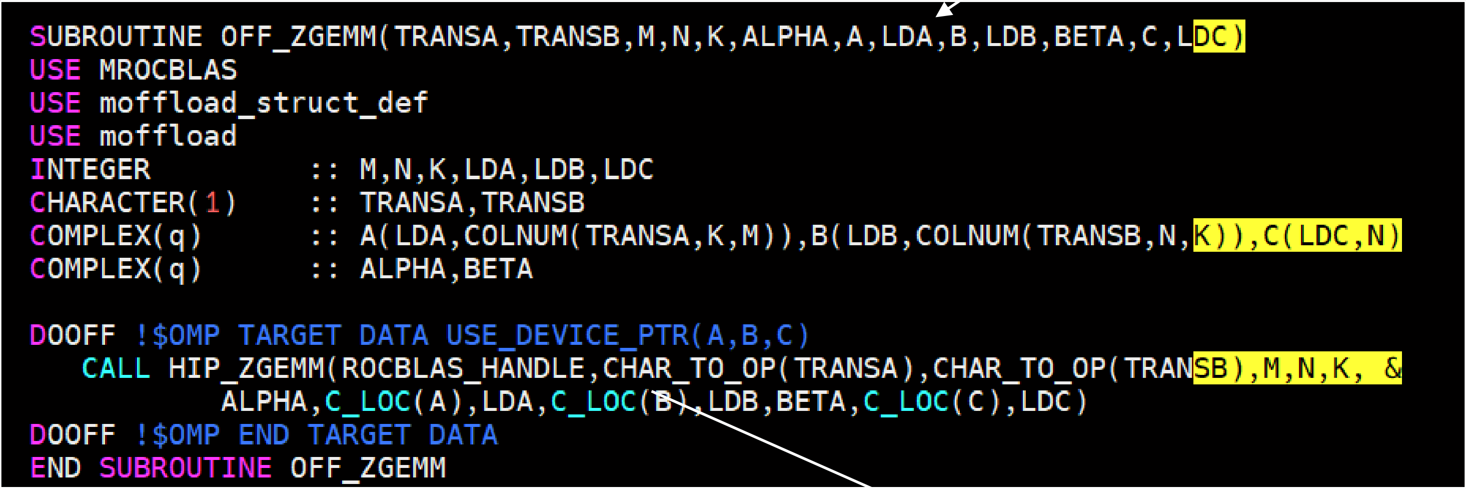
```
#include "symbol.inc"
      MODULE moffload_struct_def
#ifdef _OFFLOAD
      PUBLIC :: OMP_PUSH_EXEC_ON,OMP_POP_EXEC_ON
      INTEGER, PARAMETER :: MAXLEVEL=20
      INTEGER :: OMP_EXEC_ON_LEVEL=0
      LOGICAL :: OMP_EXEC_ON_STACK(MAXLEVEL)=.FALSE.
      LOGICAL, PUBLIC :: OMP_EXEC_ON=.TRUE.

      CONTAINS

      SUBROUTINE OMP_PUSH_EXEC_ON(VAR)
         LOGICAL :: VAR
         IF (OMP_EXEC_ON_LEVEL==MAXLEVEL) THEN
          WRITE(*,*) "OMP_PUSH_EXEC_ON: ERROR: stack is full"
         ENDIF
         OMP_EXEC_ON_LEVEL=OMP_EXEC_ON_LEVEL+1
         OMP_EXEC_ON_STACK(OMP_EXEC_ON_LEVEL)=OMP_EXEC_ON
         OMP_EXEC_ON=VAR
      END SUBROUTINE OMP_PUSH_EXEC_ON

      SUBROUTINE OMP_POP_EXEC_ON
      IF (OMP_EXEC_ON_LEVEL==0) THEN
        WRITE(*,*) "OMP_POP_EXEC_ON: ERROR: stack is empty"
      ENDIF
      OMP_EXEC_ON=OMP_EXEC_ON_STACK(OMP_EXEC_ON_LEVEL)
      OMP_EXEC_ON_LEVEL=OMP_EXEC_ON_LEVEL-1
      END SUBROUTINE OMP_POP_EXEC_ON
#endif
      END MODULE moffload_struct_def
```

Interface OMP offloading with ROCM libraries

- VASP uses FFT, BLAS, and LAPACK extensively
- Developed a wrapper to interface OMP target regions with ROCM libraries
  - rocFFT
  - rocBLAS
  - rocSolver

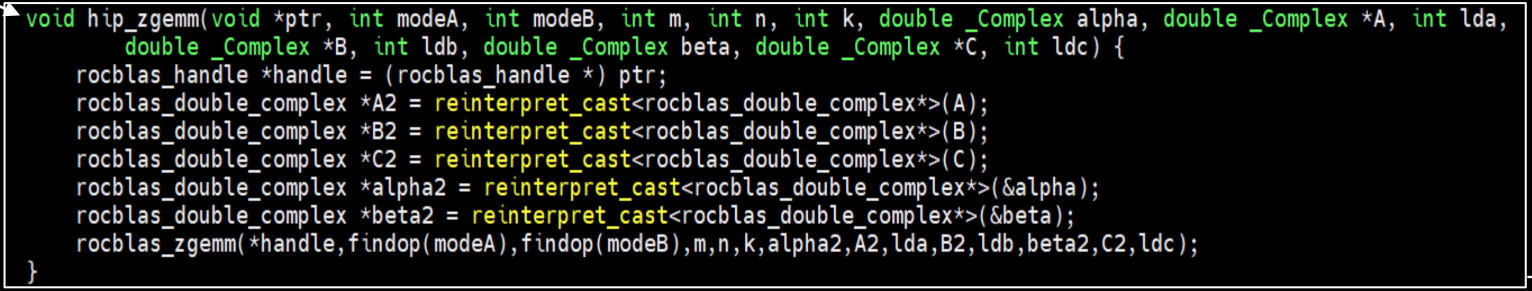


```
      CALL OFF_ZGEMM('N', 'N', m_ WDES1%NPL_RED , NSIM_, NSIM_*ITER, one, &
      &                 WOPT%CW_RED(1,1), m_ WDES%NRPLWV_RED, CEIG(1,1), NSUBD,  &
      &                 zero, WA%CW_RED(1,NPOS_RED+1), m_ WDES%NRPLWV_RED)
```



```
SUBROUTINE OFF_ZGEMM(TRANSA,TRANSB,M,N,K,ALPHA,A,LDA,B,LDB,BETA,C,LDC)
USE MROCBLAS
USE moffload_struct_def
USE moffload
INTEGER          :: M,N,K,LDA,LDB,LDC
CHARACTER(1)     :: TRANSA,TRANSB
COMPLEX(q)       :: A(LDA,COLNUM(TRANSA,K,M)),B(LDB,COLNUM(TRANSB,N,K)),C(LDC,N)
COMPLEX(q)       :: ALPHA,BETA

DOOFF !$OMP TARGET DATA USE_DEVICE_PTR(A,B,C)
   CALL HIP_ZGEMM(ROCBLAS_HANDLE,CHAR_TO_OP(TRANSA),CHAR_TO_OP(TRANSB),M,N,K, &
           ALPHA,C_LOC(A),LDA,C_LOC(B),LDB,BETA,C_LOC(C),LDC)
DOOFF !$OMP END TARGET DATA
END SUBROUTINE OFF_ZGEMM
```

WOPT%CW_RED(A), CEIG(B), and WA%CW_RED(C) are mapped to device with “omp target enter data map” directive



```
void hip_zgemm(void *ptr, int modeA, int modeB, int m, int n, int k, double _Complex alpha, double _Complex *A, int lda,
        double _Complex *B, int ldb, double _Complex beta, double _Complex *C, int ldc) {
    rocblas_handle *handle = (rocblas_handle *) ptr;
    rocblas_double_complex *A2 = reinterpret_cast<rocblas_double_complex*>(A);
    rocblas_double_complex *B2 = reinterpret_cast<rocblas_double_complex*>(B);
    rocblas_double_complex *C2 = reinterpret_cast<rocblas_double_complex*>(C);
    rocblas_double_complex *alpha2 = reinterpret_cast<rocblas_double_complex*>(&alpha);
    rocblas_double_complex *beta2 = reinterpret_cast<rocblas_double_complex*>(&beta);
    rocblas_zgemm(*handle,findop(modeA),findop(modeB),m,n,k,alpha2,A2,lda,B2,ldb,beta2,C2,ldc);
}
```

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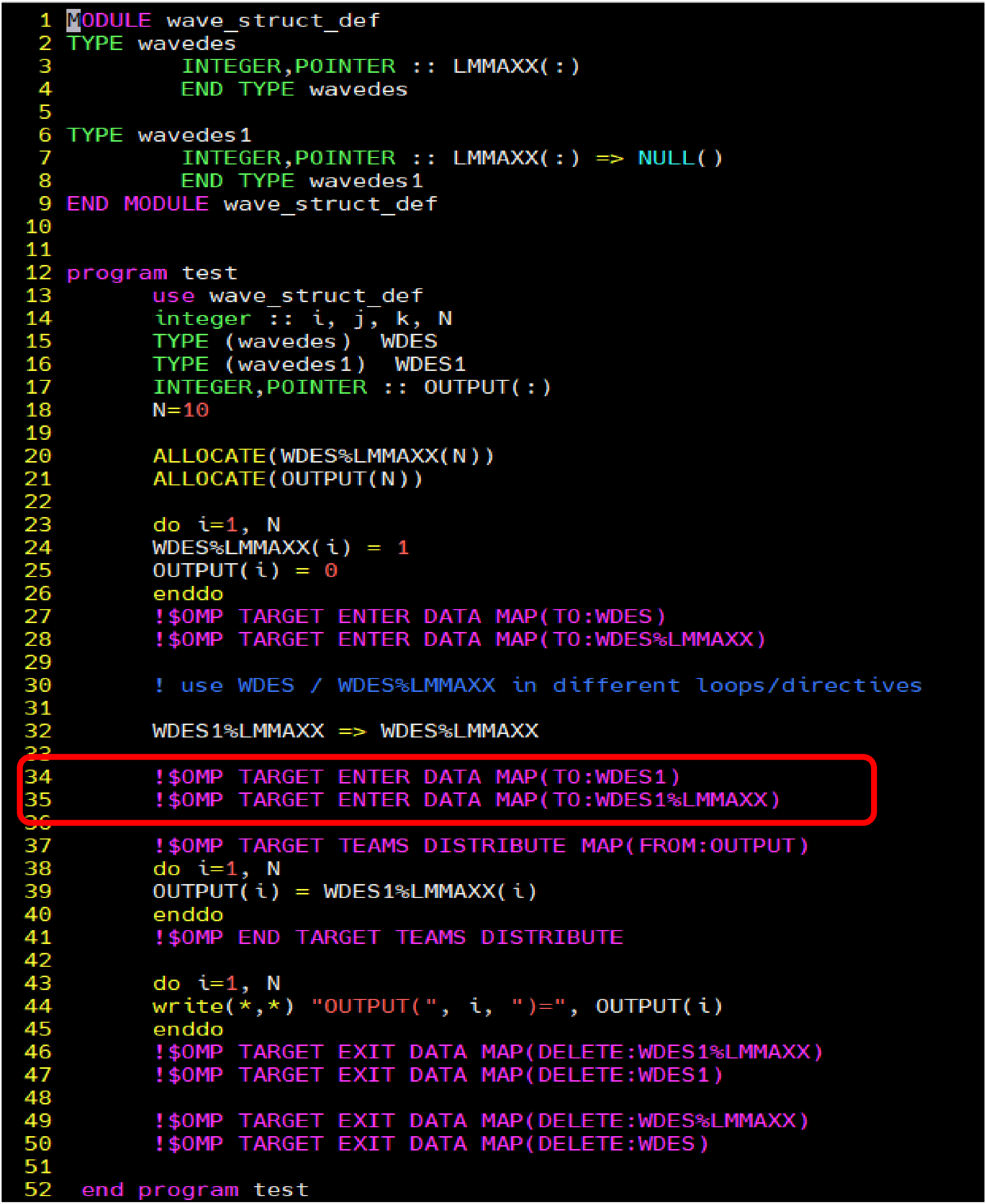
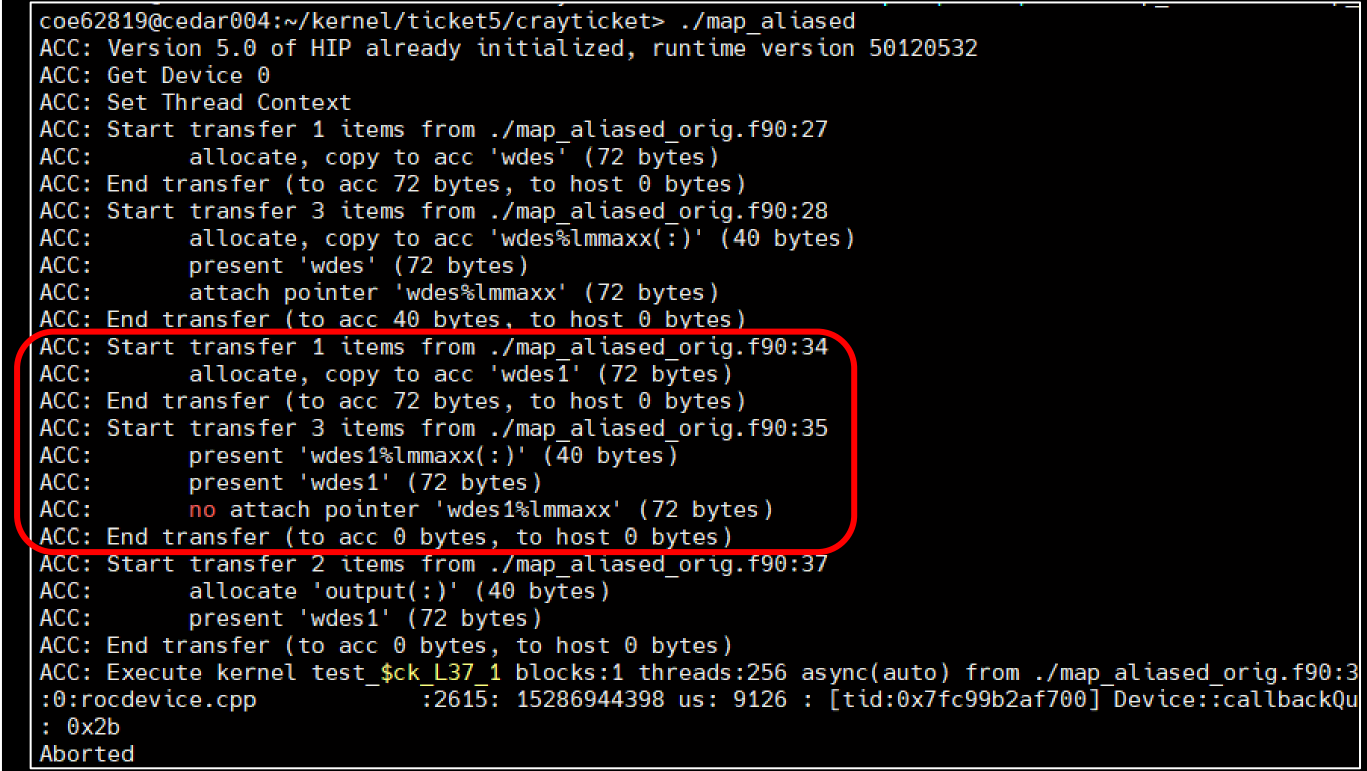
Pointer aliasing



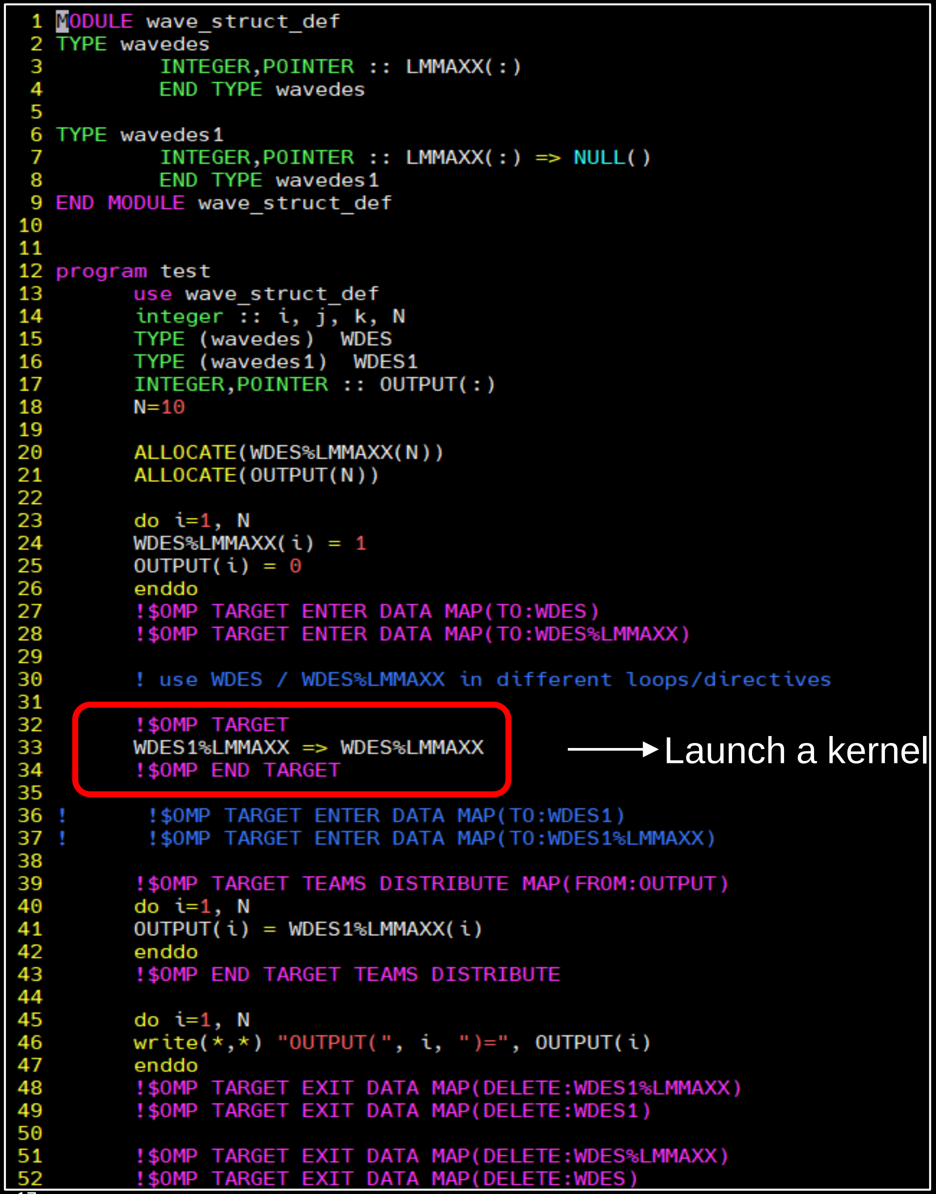
```
 1 MODULE wave_struct_def
 2 TYPE wavedes
 3         INTEGER,POINTER :: LMMAXX(:)
 4         END TYPE wavedes
 5
 6 TYPE wavedes1
 7         INTEGER,POINTER :: LMMAXX(:) => NULL()
 8         END TYPE wavedes1
 9 END MODULE wave_struct_def
10
11
12 program test
13       use wave_struct_def
14       integer :: i, j, k, N
15       TYPE (wavedes)  WDES
16       TYPE (wavedes1)  WDES1
17       INTEGER,POINTER :: OUTPUT(:)
18       N=10
19
20       ALLOCATE(WDES%LMMAXX(N))
21       ALLOCATE(OUTPUT(N))
22
23       do i=1, N
24       WDES%LMMAXX(i) = 1
25       OUTPUT(i) = 0
26       enddo
27       !$OMP TARGET ENTER DATA MAP(TO:WDES)
28       !$OMP TARGET ENTER DATA MAP(TO:WDES%LMMAXX)
29
30       ! use WDES / WDES%LMMAXX in different loops/directives
31
32       WDES1%LMMAXX => WDES%LMMAXX
33
34       !$OMP TARGET ENTER DATA MAP(TO:WDES1)
35       !$OMP TARGET ENTER DATA MAP(TO:WDES1%LMMAXX)
36
37       !$OMP TARGET TEAMS DISTRIBUTE MAP(FROM:OUTPUT)
38       do i=1, N
39       OUTPUT(i) = WDES1%LMMAXX(i)
40       enddo
41       !$OMP END TARGET TEAMS DISTRIBUTE
42
43       do i=1, N
44       write(*,*) "OUTPUT(", i, ")=", OUTPUT(i)
45       enddo
46       !$OMP TARGET EXIT DATA MAP(DELETE:WDES1%LMMAXX)
47       !$OMP TARGET EXIT DATA MAP(DELETE:WDES1)
48
49       !$OMP TARGET EXIT DATA MAP(DELETE:WDES%LMMAXX)
50       !$OMP TARGET EXIT DATA MAP(DELETE:WDES)
51
52  end program test
```

- Pointer aliasing occurs a lot in VASP
  - It can be challenging for the compilers to deal with pointer aliasing on device
- Set CRAY_ACC_DEBUG=3 as environment variable to get the log
- This issue is resolved in CCE15



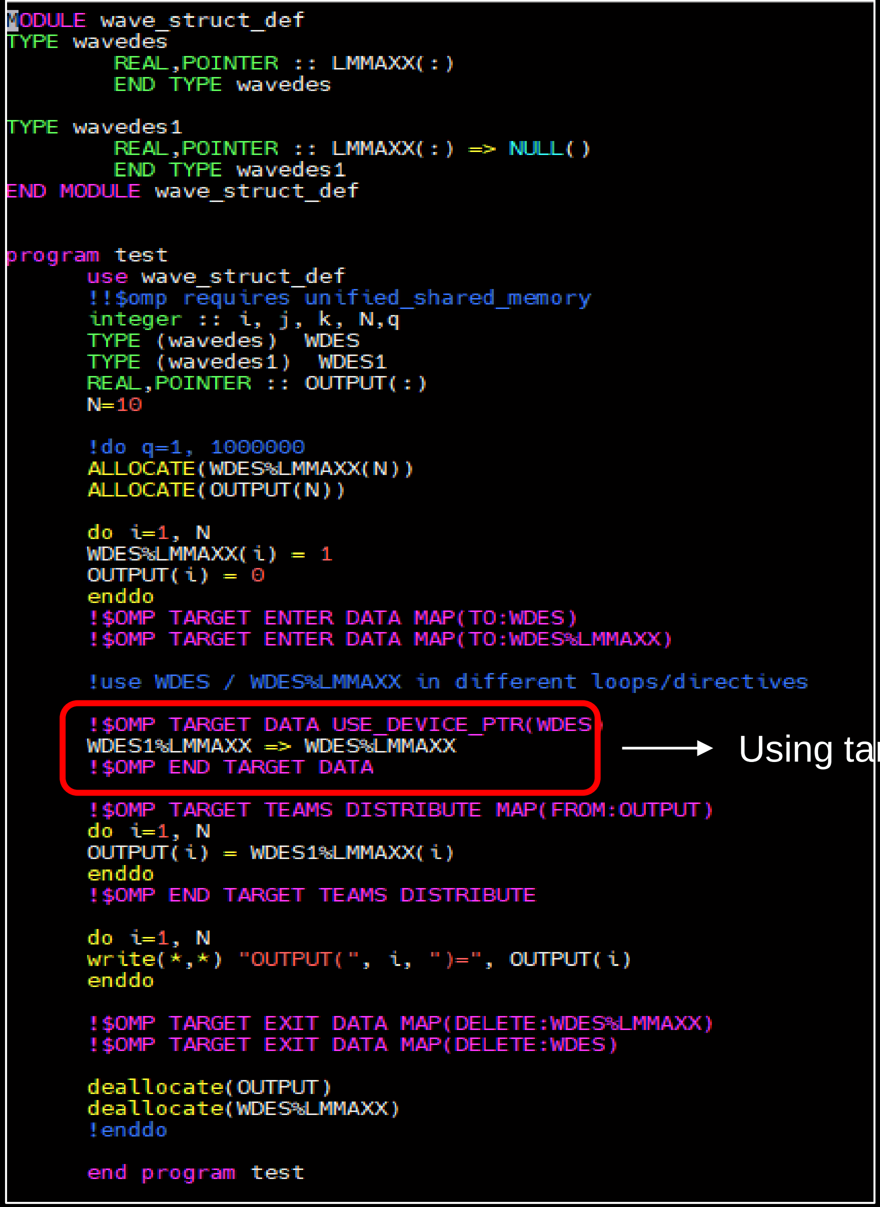
```
coe62819@cedar004:~/kernel/ticket5/crayticket> ./map_aliased
ACC: Version 5.0 of HIP already initialized, runtime version 50120532
ACC: Get Device 0
ACC: Set Thread Context
ACC: Start transfer 1 items from ./map_aliased_orig.f90:27
ACC:        allocate, copy to acc 'wdes' (72 bytes)
ACC: End transfer (to acc 72 bytes, to host 0 bytes)
ACC: Start transfer 3 items from ./map_aliased_orig.f90:28
ACC:        allocate, copy to acc 'wdes%lmmaxx(:)' (40 bytes)
ACC:        present 'wdes' (72 bytes)
ACC:        attach pointer 'wdes%lmmaxx' (72 bytes)
ACC: End transfer (to acc 40 bytes, to host 0 bytes)
ACC: Start transfer 1 items from ./map_aliased_orig.f90:34
ACC:        allocate, copy to acc 'wdes1' (72 bytes)
ACC: End transfer (to acc 72 bytes, to host 0 bytes)
ACC: Start transfer 3 items from ./map_aliased_orig.f90:35
ACC:        present 'wdes1%lmmaxx(:)' (40 bytes)
ACC:        present 'wdes1' (72 bytes)
ACC:        no attach pointer 'wdes1%lmmaxx' (72 bytes)
ACC: End transfer (to acc 0 bytes, to host 0 bytes)
ACC: Start transfer 2 items from ./map_aliased_orig.f90:37
ACC:        allocate 'output(:)' (40 bytes)
ACC:        present 'wdes1' (72 bytes)
ACC: End transfer (to acc 0 bytes, to host 0 bytes)
ACC: Execute kernel test_$ck_L37_1 blocks:1 threads:256 async(auto) from ./map_aliased_orig.f90:3
:0:rocdevice.cpp            :2615: 15286944398 us: 9126 : [tid:0x7fc99b2af700] Device::callbackQu
: 0x2b
Aborted
```

Pointer aliasing (alternative methods)



```
MODULE wave_struct_def
TYPE wavedes
        INTEGER,POINTER :: LMMAXX(:)
        END TYPE wavedes

TYPE wavedes1
        INTEGER,POINTER :: LMMAXX(:) => NULL()
        END TYPE wavedes1
END MODULE wave_struct_def


program test
      use wave_struct_def
      integer :: i, j, k, N
      TYPE (wavedes)  WDES
      TYPE (wavedes1)  WDES1
      INTEGER,POINTER :: OUTPUT(:)
      N=10

      ALLOCATE(WDES%LMMAXX(N))
      ALLOCATE(OUTPUT(N))

      do i=1, N
      WDES%LMMAXX(i) = 1
      OUTPUT(i) = 0
      enddo
      !$OMP TARGET ENTER DATA MAP(TO:WDES)
      !$OMP TARGET ENTER DATA MAP(TO:WDES%LMMAXX)

      ! use WDES / WDES%LMMAXX in different loops/directives

      !$OMP TARGET
      WDES1%LMMAXX => WDES%LMMAXX
      !$OMP END TARGET

!      !$OMP TARGET ENTER DATA MAP(TO:WDES1)
!      !$OMP TARGET ENTER DATA MAP(TO:WDES1%LMMAXX)

      !$OMP TARGET TEAMS DISTRIBUTE MAP(FROM:OUTPUT)
      do i=1, N
      OUTPUT(i) = WDES1%LMMAXX(i)
      enddo
      !$OMP END TARGET TEAMS DISTRIBUTE

      do i=1, N
      write(*,*) "OUTPUT(", i, ")=", OUTPUT(i)
      enddo
      !$OMP TARGET EXIT DATA MAP(DELETE:WDES1%LMMAXX)
      !$OMP TARGET EXIT DATA MAP(DELETE:WDES1)

      !$OMP TARGET EXIT DATA MAP(DELETE:WDES%LMMAXX)
      !$OMP TARGET EXIT DATA MAP(DELETE:WDES)
```

→ Launch a kernel

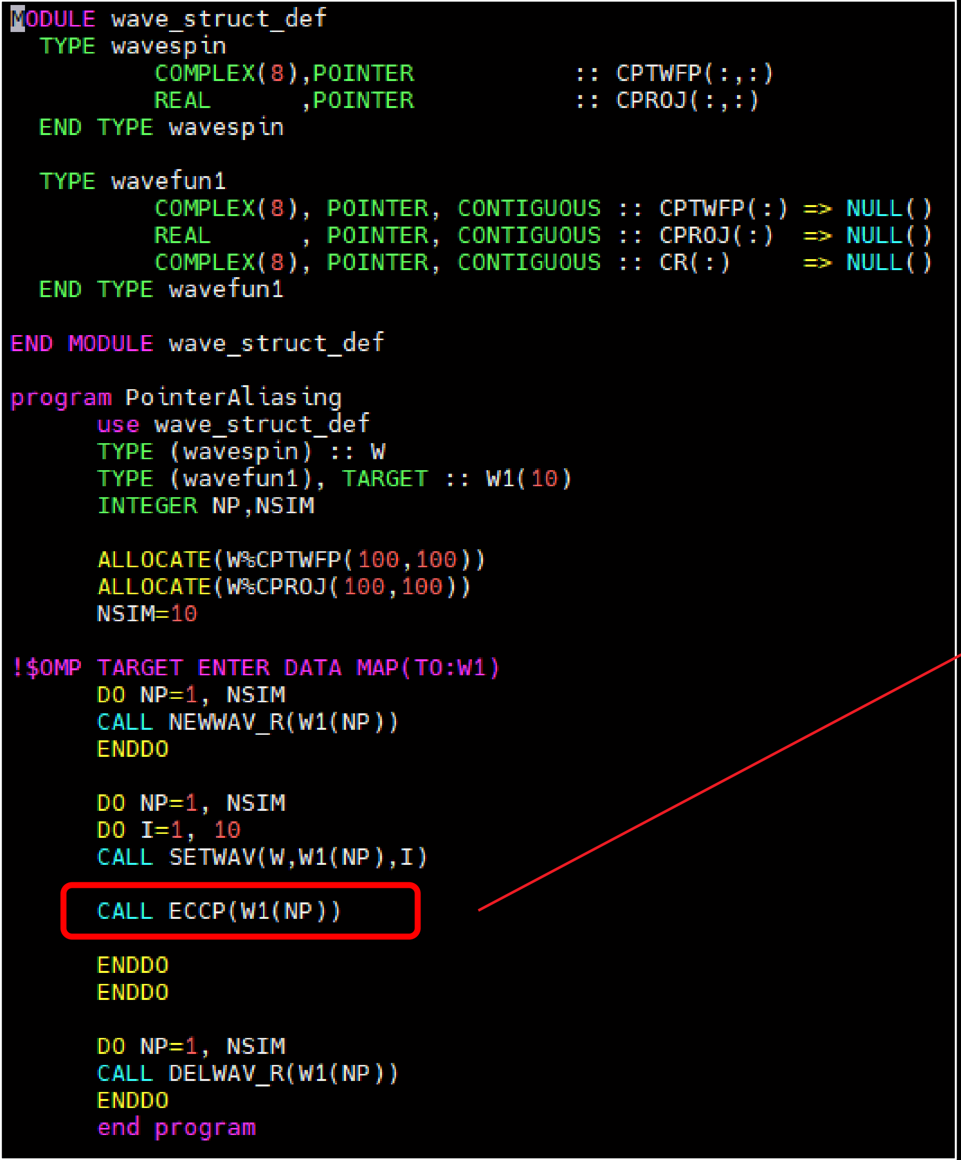


```
MODULE wave_struct_def
TYPE wavedes
        REAL,POINTER :: LMMAXX(:)
        END TYPE wavedes

TYPE wavedes1
        REAL,POINTER :: LMMAXX(:) => NULL()
        END TYPE wavedes1
END MODULE wave_struct_def


program test
      use wave_struct_def
      !!$omp requires unified_shared_memory
      integer :: i, j, k, N,q
      TYPE (wavedes)  WDES
      TYPE (wavedes1)  WDES1
      REAL,POINTER :: OUTPUT(:)
      N=10

      !do q=1, 1000000
      ALLOCATE(WDES%LMMAXX(N))
      ALLOCATE(OUTPUT(N))

      do i=1, N
      WDES%LMMAXX(i) = 1
      OUTPUT(i) = 0
      enddo
      !$OMP TARGET ENTER DATA MAP(TO:WDES)
      !$OMP TARGET ENTER DATA MAP(TO:WDES%LMMAXX)

      !use WDES / WDES%LMMAXX in different loops/directives

      !$OMP TARGET DATA USE_DEVICE_PTR(WDES)
      WDES1%LMMAXX => WDES%LMMAXX
      !$OMP END TARGET DATA

      !$OMP TARGET TEAMS DISTRIBUTE MAP(FROM:OUTPUT)
      do i=1, N
      OUTPUT(i) = WDES1%LMMAXX(i)
      enddo
      !$OMP END TARGET TEAMS DISTRIBUTE

      do i=1, N
      write(*,*) "OUTPUT(", i, ")=", OUTPUT(i)
      enddo

      !$OMP TARGET EXIT DATA MAP(DELETE:WDES%LMMAXX)
      !$OMP TARGET EXIT DATA MAP(DELETE:WDES)

      deallocate(OUTPUT)
      deallocate(WDES%LMMAXX)
      !enddo

      end program test
```

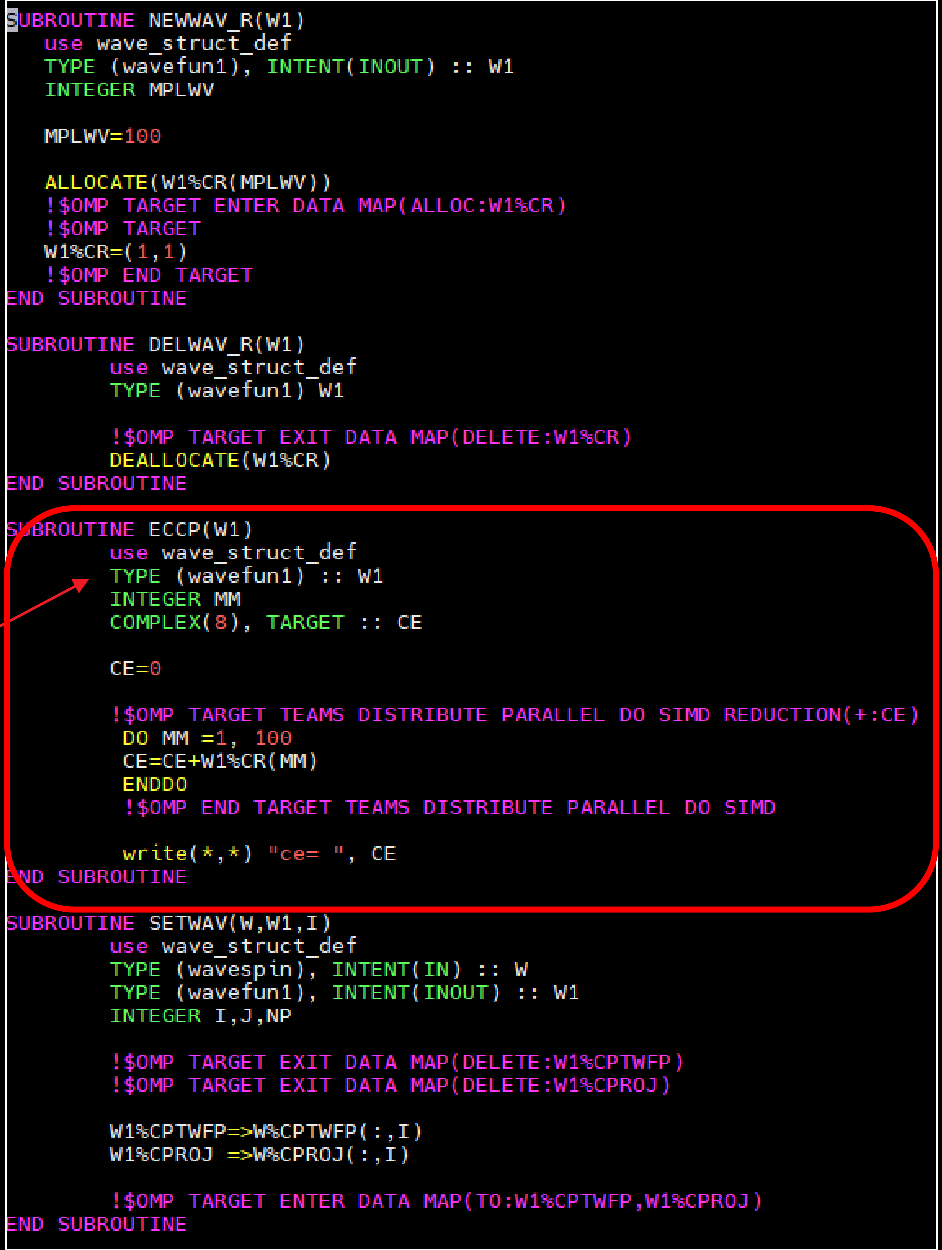
→ Using target data construct

AMD
together we advance_

Pointer mismatch in subroutine calls



```fortran
MODULE wave_struct_def
  TYPE wavespin
          COMPLEX(8),POINTER             :: CPTWFP(:,:)
          REAL      ,POINTER             :: CPROJ(:,:)
  END TYPE wavespin

  TYPE wavefun1
          COMPLEX(8), POINTER, CONTIGUOUS :: CPTWFP(:) => NULL()
          REAL      , POINTER, CONTIGUOUS :: CPROJ(:)  => NULL()
          COMPLEX(8), POINTER, CONTIGUOUS :: CR(:)     => NULL()
  END TYPE wavefun1

END MODULE wave_struct_def

program PointerAliasing
      use wave_struct_def
      TYPE (wavespin) :: W
      TYPE (wavefun1), TARGET :: W1(10)
      INTEGER NP,NSIM

      ALLOCATE(W%CPTWFP(100,100))
      ALLOCATE(W%CPROJ(100,100))
      NSIM=10

!$OMP TARGET ENTER DATA MAP(TO:W1)
      DO NP=1, NSIM
      CALL NEWWAV_R(W1(NP))
      ENDDO

      DO NP=1, NSIM
      DO I=1, 10
      CALL SETWAV(W,W1(NP),I)

      CALL ECCP(W1(NP))

      ENDDO
      ENDDO

      DO NP=1, NSIM
      CALL DELWAV_R(W1(NP))
      ENDDO
      end program
```

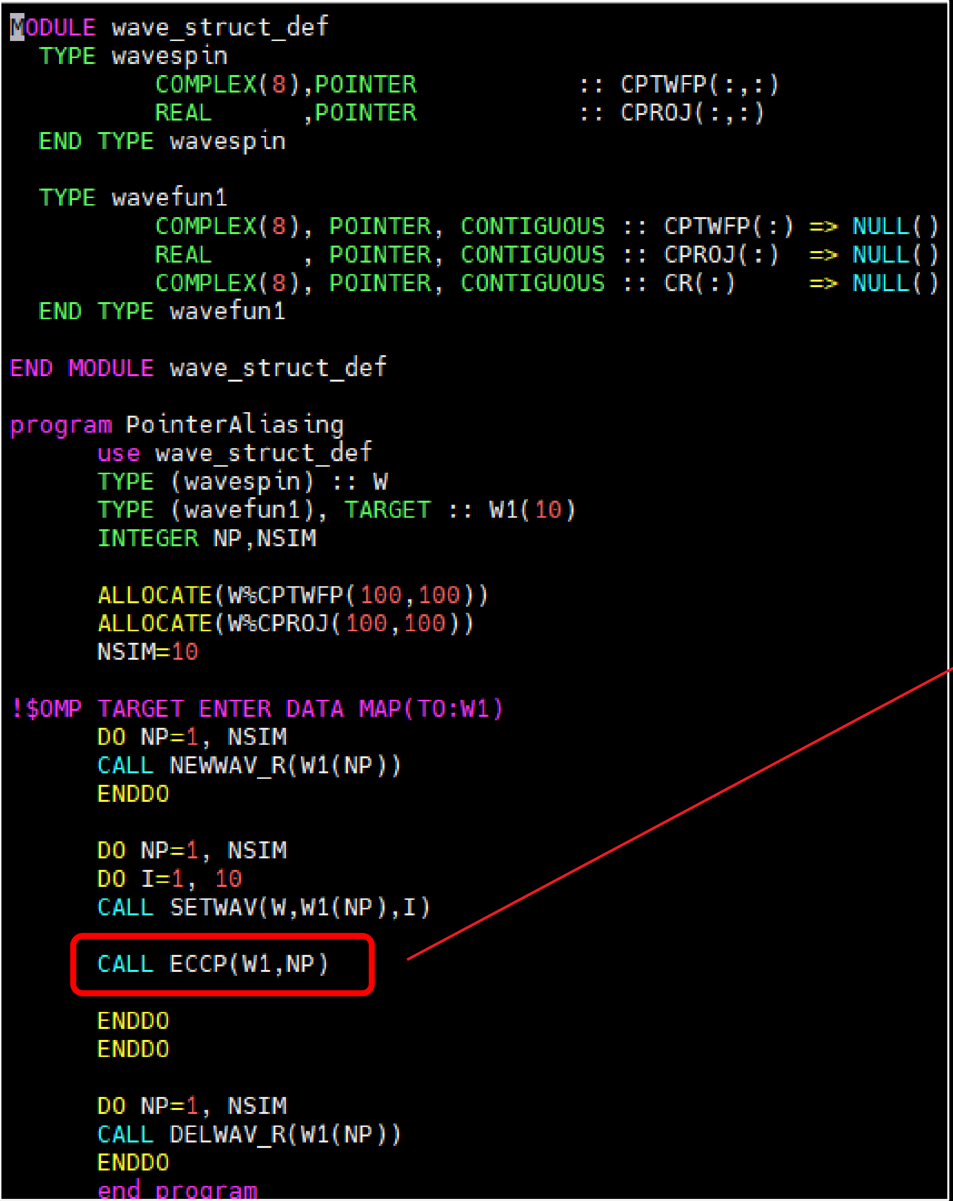


```fortran
SUBROUTINE NEWWAV_R(W1)
   use wave_struct_def
   TYPE (wavefun1), INTENT(INOUT) :: W1
   INTEGER MPLWV

   MPLWV=100

   ALLOCATE(W1%CR(MPLWV))
   !$OMP TARGET ENTER DATA MAP(ALLOC:W1%CR)
   !$OMP TARGET
   W1%CR=(1,1)
   !$OMP END TARGET
END SUBROUTINE

SUBROUTINE DELWAV_R(W1)
        use wave_struct_def
        TYPE (wavefun1) W1

        !$OMP TARGET EXIT DATA MAP(DELETE:W1%CR)
        DEALLOCATE(W1%CR)
END SUBROUTINE

SUBROUTINE ECCP(W1)
        use wave_struct_def
        TYPE (wavefun1) :: W1
        INTEGER MM
        COMPLEX(8), TARGET :: CE

        CE=0

        !$OMP TARGET TEAMS DISTRIBUTE PARALLEL DO SIMD REDUCTION(+:CE)
         DO MM =1, 100
         CE=CE+W1%CR(MM)
         ENDDO
         !$OMP END TARGET TEAMS DISTRIBUTE PARALLEL DO SIMD

         write(*,*) "ce= ", CE
END SUBROUTINE
SUBROUTINE SETWAV(W,W1,I)
        use wave_struct_def
        TYPE (wavespin), INTENT(IN) :: W
        TYPE (wavefun1), INTENT(INOUT) :: W1
        INTEGER I,J,NP

        !$OMP TARGET EXIT DATA MAP(DELETE:W1%CPTWFP)
        !$OMP TARGET EXIT DATA MAP(DELETE:W1%CPROJ)

        W1%CPTWFP=>W%CPTWFP(:,I)
        W1%CPROJ =>W%CPROJ(:,I)

        !$OMP TARGET ENTER DATA MAP(TO:W1%CPTWFP,W1%CPROJ)
END SUBROUTINE
```

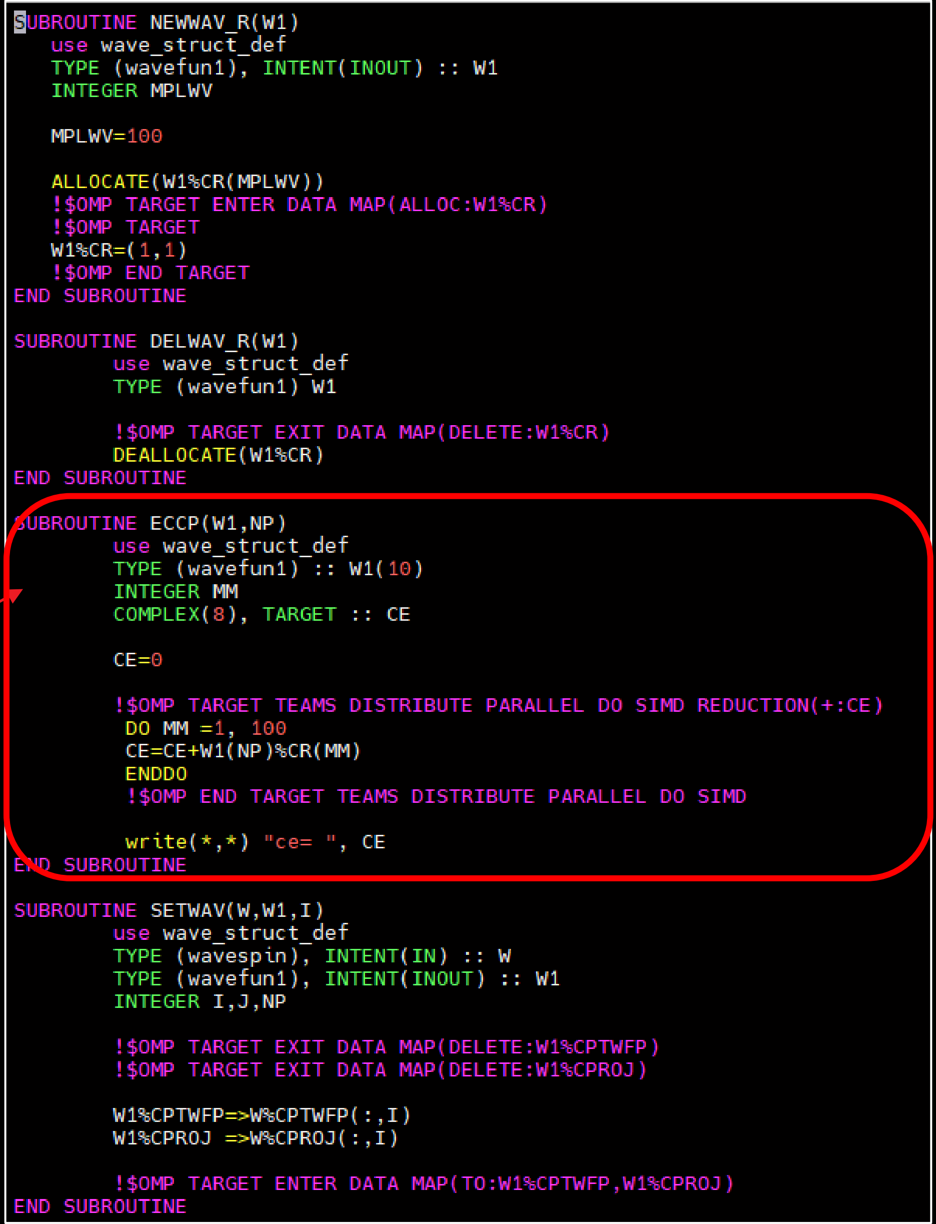
```
$./aliasing
 ce=  (100.,100.)
 ce=  (100.,100.)
 ce=  (100.,100.)
 ce=  (100.,100.)
 ce=  (100.,100.)
 ce=  (100.,100.)
 ce=  (100.,100.)
 ce=  (100.,100.)
 ce=  (100.,100.)
 ce=  (100.,100.)
:0:rocdevice.cpp           :2660: 1637590862517 us:
86531: [tid:0x7fbe82217700]
Device::callbackQueue aborting with error :
HSA_STATUS_ERROR_MEMORY_APERTURE_V
IOLATION: The agent attempted to access memory
beyond the largest legal address. code: 0x29
Aborted
```

AMD
together we advance_

Pointer mismatch in subroutine calls (alternative method)

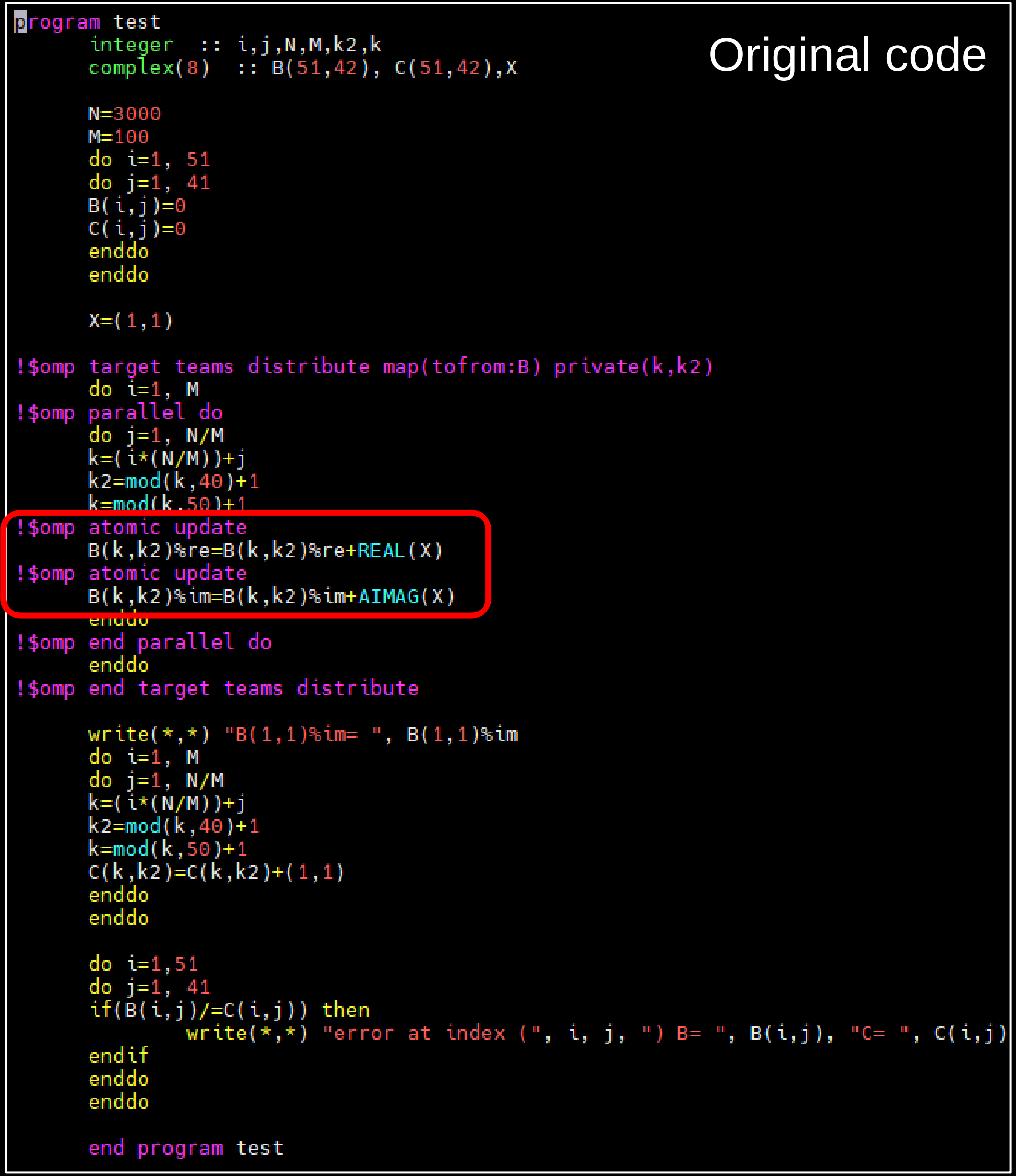


```
MODULE wave_struct_def
  TYPE wavespin
          COMPLEX(8),POINTER           :: CPTWFP(:,:)
          REAL      ,POINTER           :: CPROJ(:,:)
  END TYPE wavespin

  TYPE wavefun1
          COMPLEX(8), POINTER, CONTIGUOUS :: CPTWFP(:) => NULL()
          REAL      , POINTER, CONTIGUOUS :: CPROJ(:)  => NULL()
          COMPLEX(8), POINTER, CONTIGUOUS :: CR(:)     => NULL()
  END TYPE wavefun1

END MODULE wave_struct_def

program PointerAliasing
      use wave_struct_def
      TYPE (wavespin) :: W
      TYPE (wavefun1), TARGET :: W1(10)
      INTEGER NP,NSIM

      ALLOCATE(W%CPTWFP(100,100))
      ALLOCATE(W%CPROJ(100,100))
      NSIM=10

!$OMP TARGET ENTER DATA MAP(TO:W1)
      DO NP=1, NSIM
      CALL NEWWAV_R(W1(NP))
      ENDDO

      DO NP=1, NSIM
      DO I=1, 10
      CALL SETWAV(W,W1(NP),I)

      CALL ECCP(W1,NP)

      ENDDO
      ENDDO

      DO NP=1, NSIM
      CALL DELWAV_R(W1(NP))
      ENDDO
      end program
```



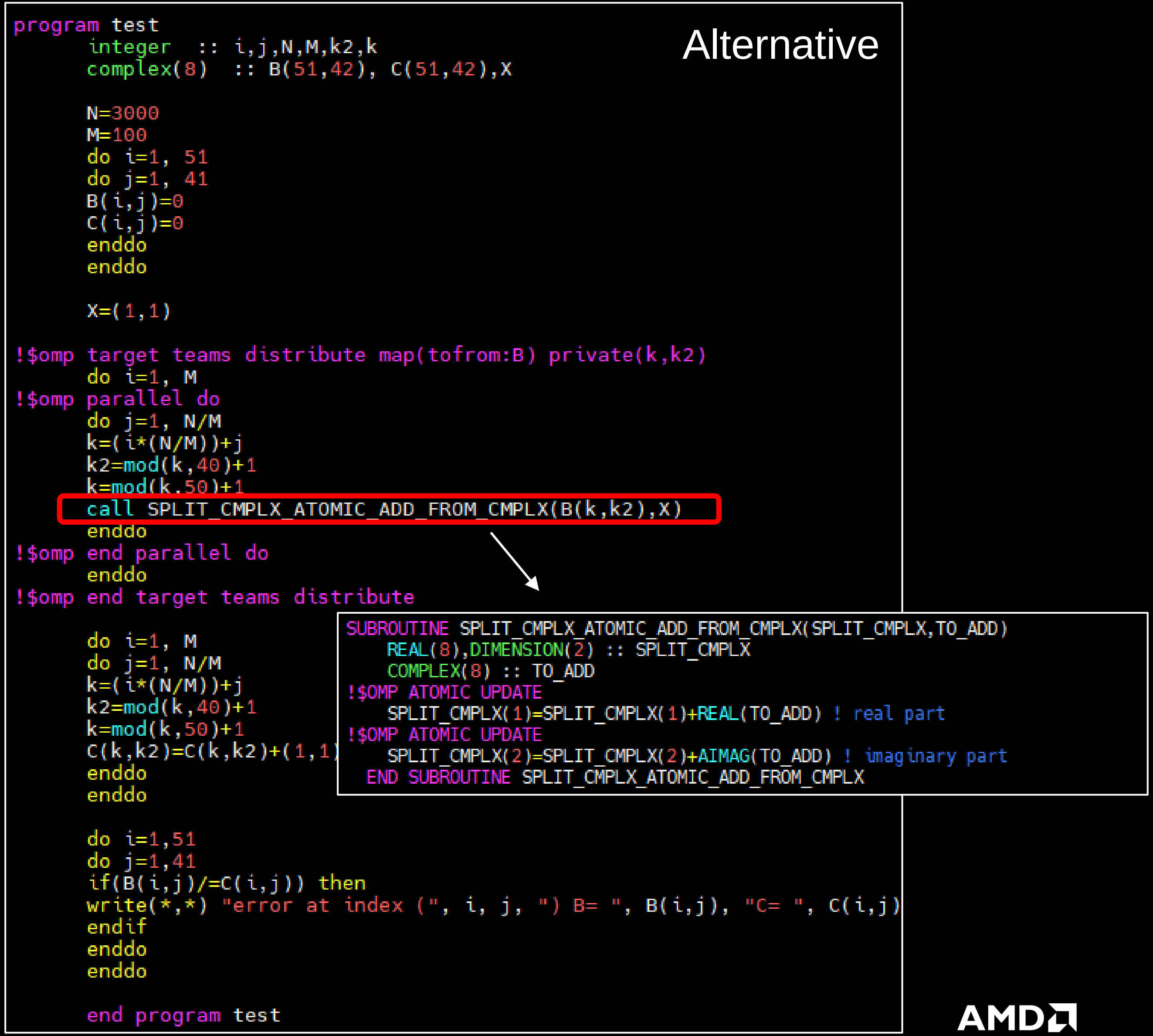
```
SUBROUTINE NEWWAV_R(W1)
   use wave_struct_def
   TYPE (wavefun1), INTENT(INOUT) :: W1
   INTEGER MPLWV

   MPLWV=100

   ALLOCATE(W1%CR(MPLWV))
   !$OMP TARGET ENTER DATA MAP(ALLOC:W1%CR)
   !$OMP TARGET
   W1%CR=(1,1)
   !$OMP END TARGET
END SUBROUTINE

SUBROUTINE DELWAV_R(W1)
        use wave_struct_def
        TYPE (wavefun1) W1

        !$OMP TARGET EXIT DATA MAP(DELETE:W1%CR)
        DEALLOCATE(W1%CR)
END SUBROUTINE

SUBROUTINE ECCP(W1,NP)
        use wave_struct_def
        TYPE (wavefun1) :: W1(10)
        INTEGER MM
        COMPLEX(8), TARGET :: CE

        CE=0

        !$OMP TARGET TEAMS DISTRIBUTE PARALLEL DO SIMD REDUCTION(+:CE)
         DO MM =1, 100
         CE=CE+W1(NP)%CR(MM)
         ENDDO
         !$OMP END TARGET TEAMS DISTRIBUTE PARALLEL DO SIMD

         write(*,*) "ce= ", CE
END SUBROUTINE

SUBROUTINE SETWAV(W,W1,I)
        use wave_struct_def
        TYPE (wavespin), INTENT(IN) :: W
        TYPE (wavefun1), INTENT(INOUT) :: W1
        INTEGER I,J,NP

        !$OMP TARGET EXIT DATA MAP(DELETE:W1%CPTWFP)
        !$OMP TARGET EXIT DATA MAP(DELETE:W1%CPROJ)

        W1%CPTWFP=>W%CPTWFP(:,I)
        W1%CPROJ =>W%CPROJ(:,I)

        !$OMP TARGET ENTER DATA MAP(TO:W1%CPTWFP,W1%CPROJ)
END SUBROUTINE
```

Atomic update for complex(8)



Original code

```
program test
      integer  :: i,j,N,M,k2,k
      complex(8)  :: B(51,42), C(51,42),X

      N=3000
      M=100
      do i=1, 51
      do j=1, 41
      B(i,j)=0
      C(i,j)=0
      enddo
      enddo

      X=(1,1)

!$omp target teams distribute map(tofrom:B) private(k,k2)
      do i=1, M
!$omp parallel do
      do j=1, N/M
      k=(i*(N/M))+j
      k2=mod(k,40)+1
      k=mod(k,50)+1
!$omp atomic update
      B(k,k2)%re=B(k,k2)%re+REAL(X)
!$omp atomic update
      B(k,k2)%im=B(k,k2)%im+AIMAG(X)
      enddo
!$omp end parallel do
      enddo
!$omp end target teams distribute

      write(*,*) "B(1,1)%im= ", B(1,1)%im
      do i=1, M
      do j=1, N/M
      k=(i*(N/M))+j
      k2=mod(k,40)+1
      k=mod(k,50)+1
      C(k,k2)=C(k,k2)+(1,1)
      enddo
      enddo

      do i=1,51
      do j=1, 41
      if(B(i,j)/=C(i,j)) then
             write(*,*) "error at index (", i, j, ") B= ", B(i,j), "C= ", C(i,j)
      endif
      enddo
      enddo

      end program test
```

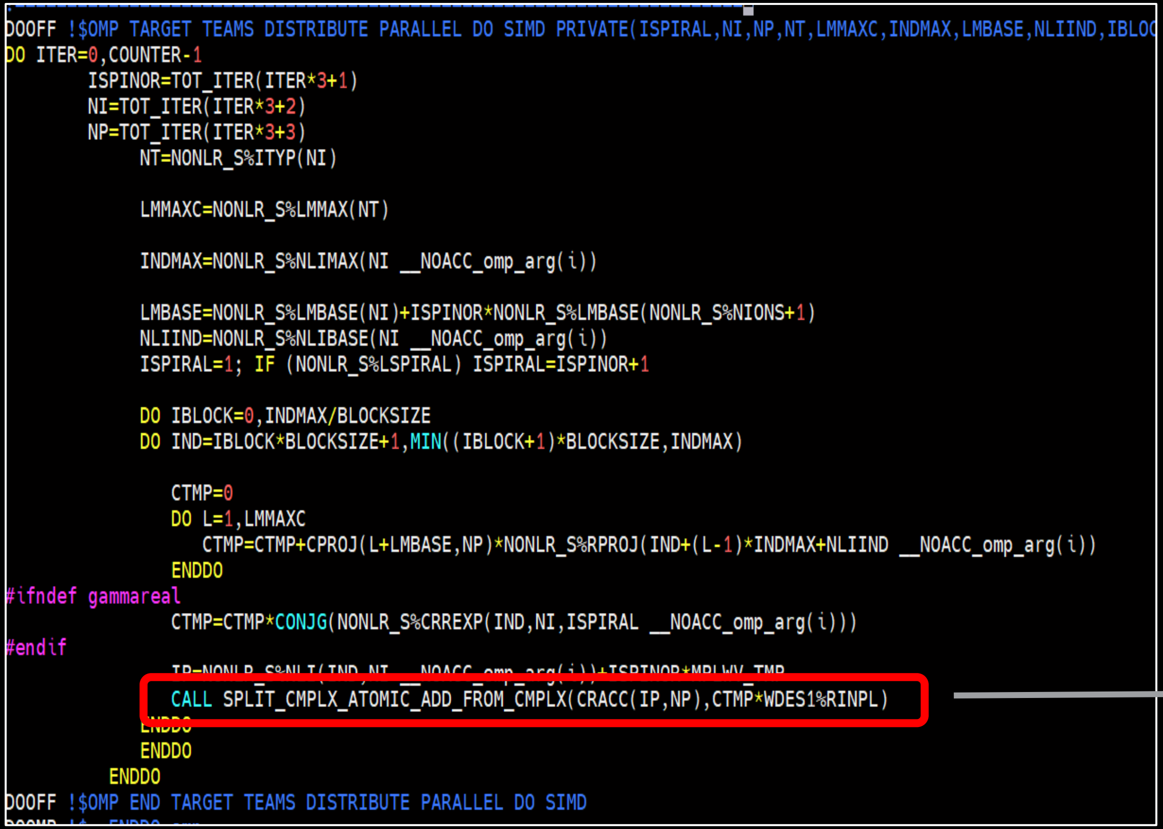


Alternative

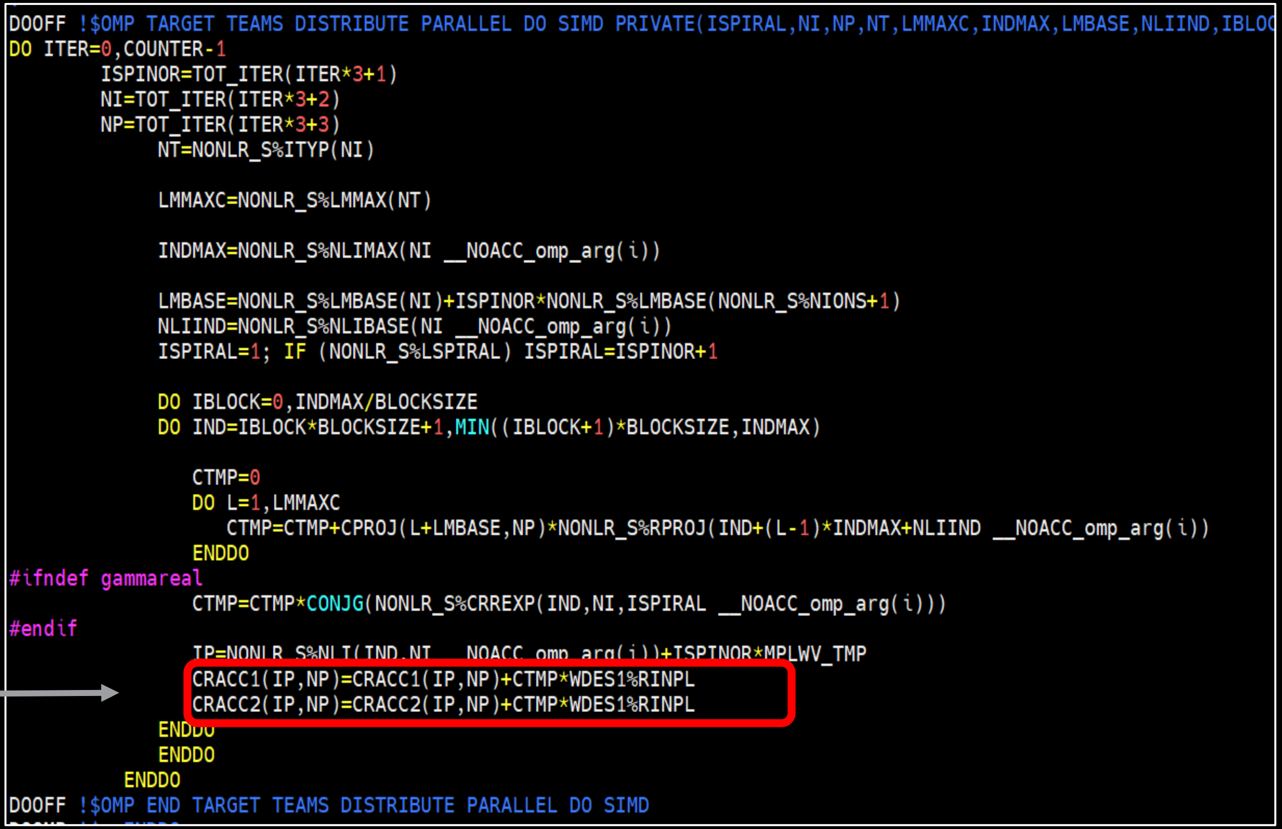
```
program test
      integer  :: i,j,N,M,k2,k
      complex(8)  :: B(51,42), C(51,42),X

      N=3000
      M=100
      do i=1, 51
      do j=1, 41
      B(i,j)=0
      C(i,j)=0
      enddo
      enddo

      X=(1,1)

!$omp target teams distribute map(tofrom:B) private(k,k2)
      do i=1, M
!$omp parallel do
      do j=1, N/M
      k=(i*(N/M))+j
      k2=mod(k,40)+1
      k=mod(k,50)+1
      call SPLIT_CMPLX_ATOMIC_ADD_FROM_CMPLX(B(k,k2),X)
      enddo
!$omp end parallel do
      enddo
!$omp end target teams distribute

      do i=1, M
      do j=1, N/M
      k=(i*(N/M))+j
      k2=mod(k,40)+1
      k=mod(k,50)+1
      C(k,k2)=C(k,k2)+(1,1)
      enddo
      enddo

      do i=1,51
      do j=1,41
      if(B(i,j)/=C(i,j)) then
      write(*,*) "error at index (", i, j, ") B= ", B(i,j), "C= ", C(i,j)
      endif
      enddo
      enddo

      end program test
```

```
SUBROUTINE SPLIT_CMPLX_ATOMIC_ADD_FROM_CMPLX(SPLIT_CMPLX,TO_ADD)
    REAL(8),DIMENSION(2) :: SPLIT_CMPLX
    COMPLEX(8) :: TO_ADD
!$OMP ATOMIC UPDATE
    SPLIT_CMPLX(1)=SPLIT_CMPLX(1)+REAL(TO_ADD) ! real part
!$OMP ATOMIC UPDATE
    SPLIT_CMPLX(2)=SPLIT_CMPLX(2)+AIMAG(TO_ADD) ! imaginary part
  END SUBROUTINE SPLIT_CMPLX_ATOMIC_ADD_FROM_CMPLX
```

The overhead of subroutine call assuming there is no need for atomic update



```
DOOFF !$OMP TARGET TEAMS DISTRIBUTE PARALLEL DO SIMD PRIVATE(ISPIRAL,NI,NP,NT,LMMAXC,INDMAX,LMBASE,NLIIND,IBLOC
DO ITER=0,COUNTER-1
        ISPINOR=TOT_ITER(ITER*3+1)
        NI=TOT_ITER(ITER*3+2)
        NP=TOT_ITER(ITER*3+3)
             NT=NONLR_S%ITYP(NI)

             LMMAXC=NONLR_S%LMMAX(NT)

             INDMAX=NONLR_S%NLIMAX(NI __NOACC_omp_arg(i))

             LMBASE=NONLR_S%LMBASE(NI)+ISPINOR*NONLR_S%LMBASE(NONLR_S%NIONS+1)
             NLIIND=NONLR_S%NLIBASE(NI __NOACC_omp_arg(i))
             ISPIRAL=1; IF (NONLR_S%LSPIRAL) ISPIRAL=ISPINOR+1

             DO IBLOCK=0,INDMAX/BLOCKSIZE
             DO IND=IBLOCK*BLOCKSIZE+1,MIN((IBLOCK+1)*BLOCKSIZE,INDMAX)

                CTMP=0
                DO L=1,LMMAXC
                   CTMP=CTMP+CPROJ(L+LMBASE,NP)*NONLR_S%RPROJ(IND+(L-1)*INDMAX+NLIIND __NOACC_omp_arg(i))
                ENDDO
#ifndef gammareal
                CTMP=CTMP*CONJG(NONLR_S%CRREXP(IND,NI,ISPIRAL __NOACC_omp_arg(i)))

#endif
                IP=NONLR_S%NLI(IND,NI __NOACC_omp_arg(i))+ISPINOR*MPLWV_TMP
                CALL SPLIT_CMPLX_ATOMIC_ADD_FROM_CMPLX(CRACC(IP,NP),CTMP*WDES1%RINPL)
             ENDDO
             ENDDO
          ENDDO
DOOFF !$OMP END TARGET TEAMS DISTRIBUTE PARALLEL DO SIMD
```

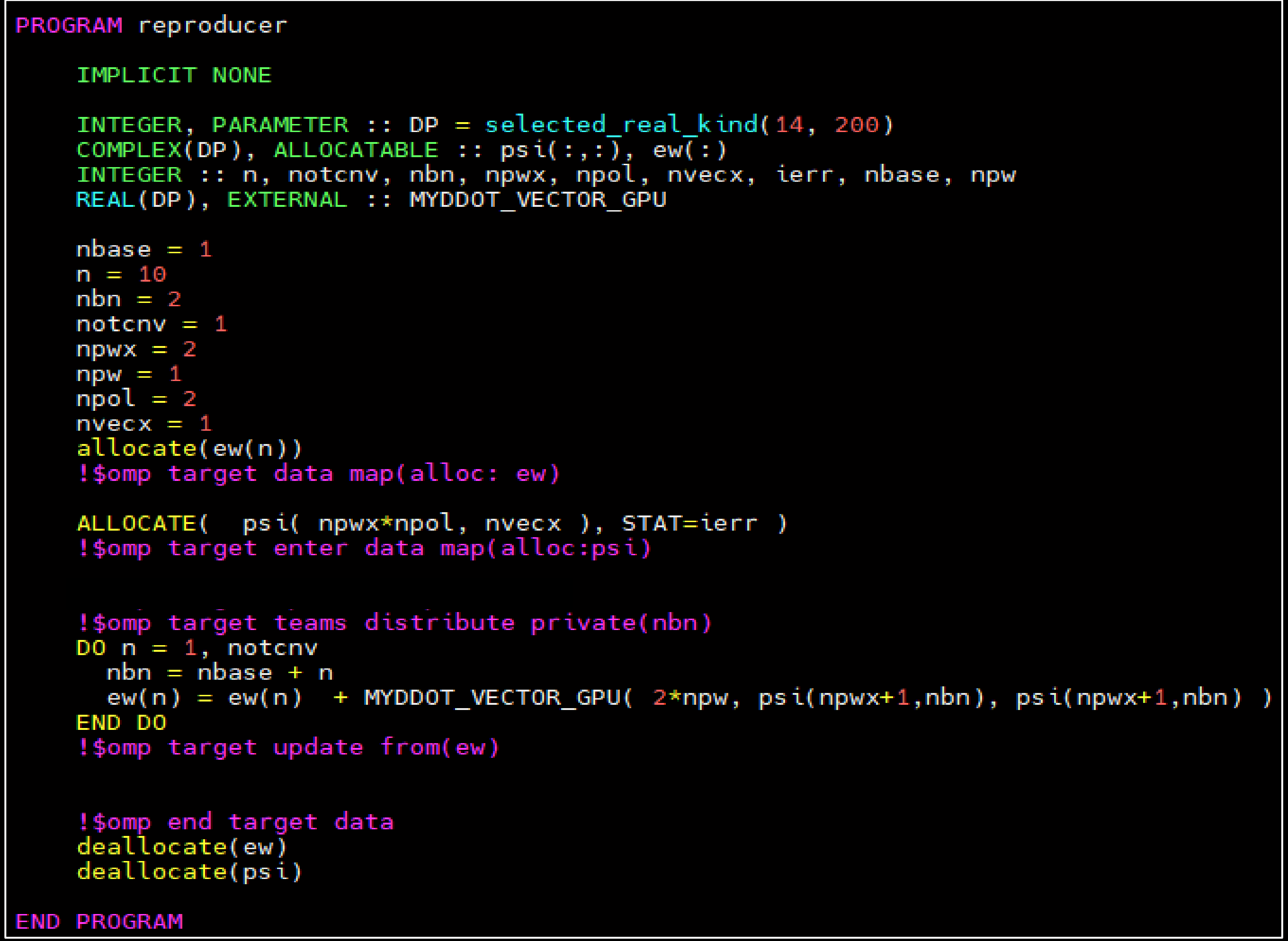


```
DOOFF !$OMP TARGET TEAMS DISTRIBUTE PARALLEL DO SIMD PRIVATE(ISPIRAL,NI,NP,NT,LMMAXC,INDMAX,LMBASE,NLIIND,IBLOC
DO ITER=0,COUNTER-1
        ISPINOR=TOT_ITER(ITER*3+1)
        NI=TOT_ITER(ITER*3+2)
        NP=TOT_ITER(ITER*3+3)
             NT=NONLR_S%ITYP(NI)

             LMMAXC=NONLR_S%LMMAX(NT)

             INDMAX=NONLR_S%NLIMAX(NI __NOACC_omp_arg(i))

             LMBASE=NONLR_S%LMBASE(NI)+ISPINOR*NONLR_S%LMBASE(NONLR_S%NIONS+1)
             NLIIND=NONLR_S%NLIBASE(NI __NOACC_omp_arg(i))
             ISPIRAL=1; IF (NONLR_S%LSPIRAL) ISPIRAL=ISPINOR+1

             DO IBLOCK=0,INDMAX/BLOCKSIZE
             DO IND=IBLOCK*BLOCKSIZE+1,MIN((IBLOCK+1)*BLOCKSIZE,INDMAX)

                CTMP=0
                DO L=1,LMMAXC
                   CTMP=CTMP+CPROJ(L+LMBASE,NP)*NONLR_S%RPROJ(IND+(L-1)*INDMAX+NLIIND __NOACC_omp_arg(i))
                ENDDO
#ifndef gammareal
                CTMP=CTMP*CONJG(NONLR_S%CRREXP(IND,NI,ISPIRAL __NOACC_omp_arg(i)))
#endif
                IP=NONLR_S%NLI(IND,NI __NOACC_omp_arg(i))+ISPINOR*MPLWV_TMP
                CRACC1(IP,NP)=CRACC1(IP,NP)+CTMP*WDES1%RINPL
                CRACC2(IP,NP)=CRACC2(IP,NP)+CTMP*WDES1%RINPL
             ENDDO
             ENDDO
          ENDDO
DOOFF !$OMP END TARGET TEAMS DISTRIBUTE PARALLEL DO SIMD
```

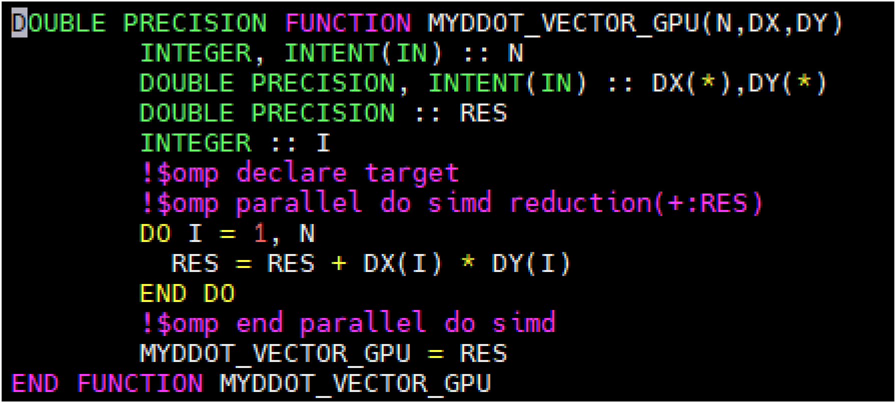
Kernel time= 80 ms

Kernel time= 22 ms

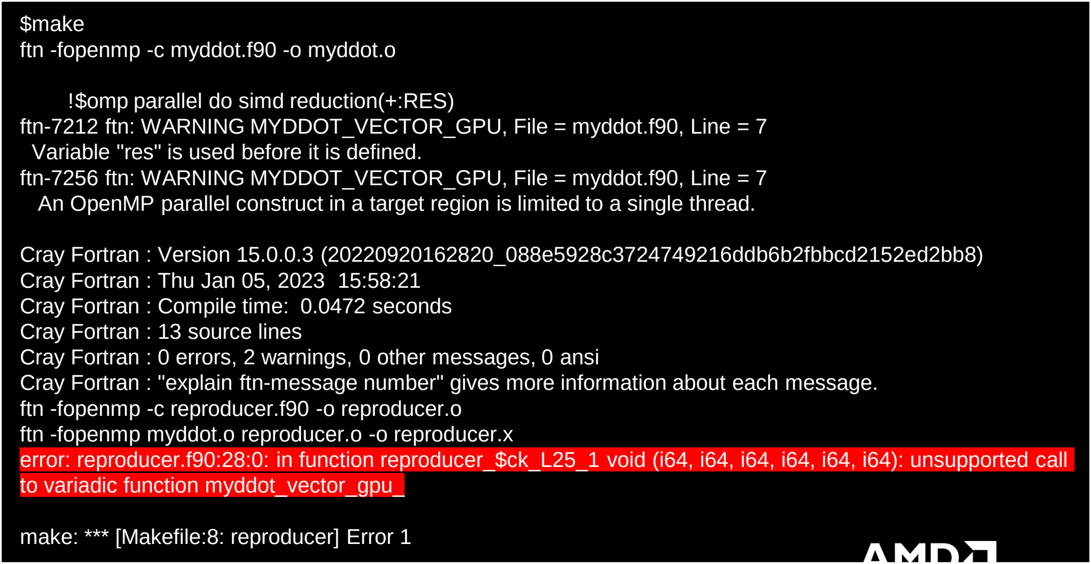
Declare target



```fortran
PROGRAM reproducer

    IMPLICIT NONE

    INTEGER, PARAMETER :: DP = selected_real_kind(14, 200)
    COMPLEX(DP), ALLOCATABLE :: psi(:,:), ew(:)
    INTEGER :: n, notcnv, nbn, npwx, npol, nvecx, ierr, nbase, npw
    REAL(DP), EXTERNAL :: MYDDOT_VECTOR_GPU

    nbase = 1
    n = 10
    nbn = 2
    notcnv = 1
    npwx = 2
    npw = 1
    npol = 2
    nvecx = 1
    allocate(ew(n))
    !$omp target data map(alloc: ew)

    ALLOCATE(  psi( npwx*npol, nvecx ), STAT=ierr )
    !$omp target enter data map(alloc:psi)


    !$omp target teams distribute private(nbn)
    DO n = 1, notcnv
      nbn = nbase + n
      ew(n) = ew(n)  + MYDDOT_VECTOR_GPU( 2*npw, psi(npwx+1,nbn), psi(npwx+1,nbn) )
    END DO
    !$omp target update from(ew)


    !$omp end target data
    deallocate(ew)
    deallocate(psi)

END PROGRAM
```

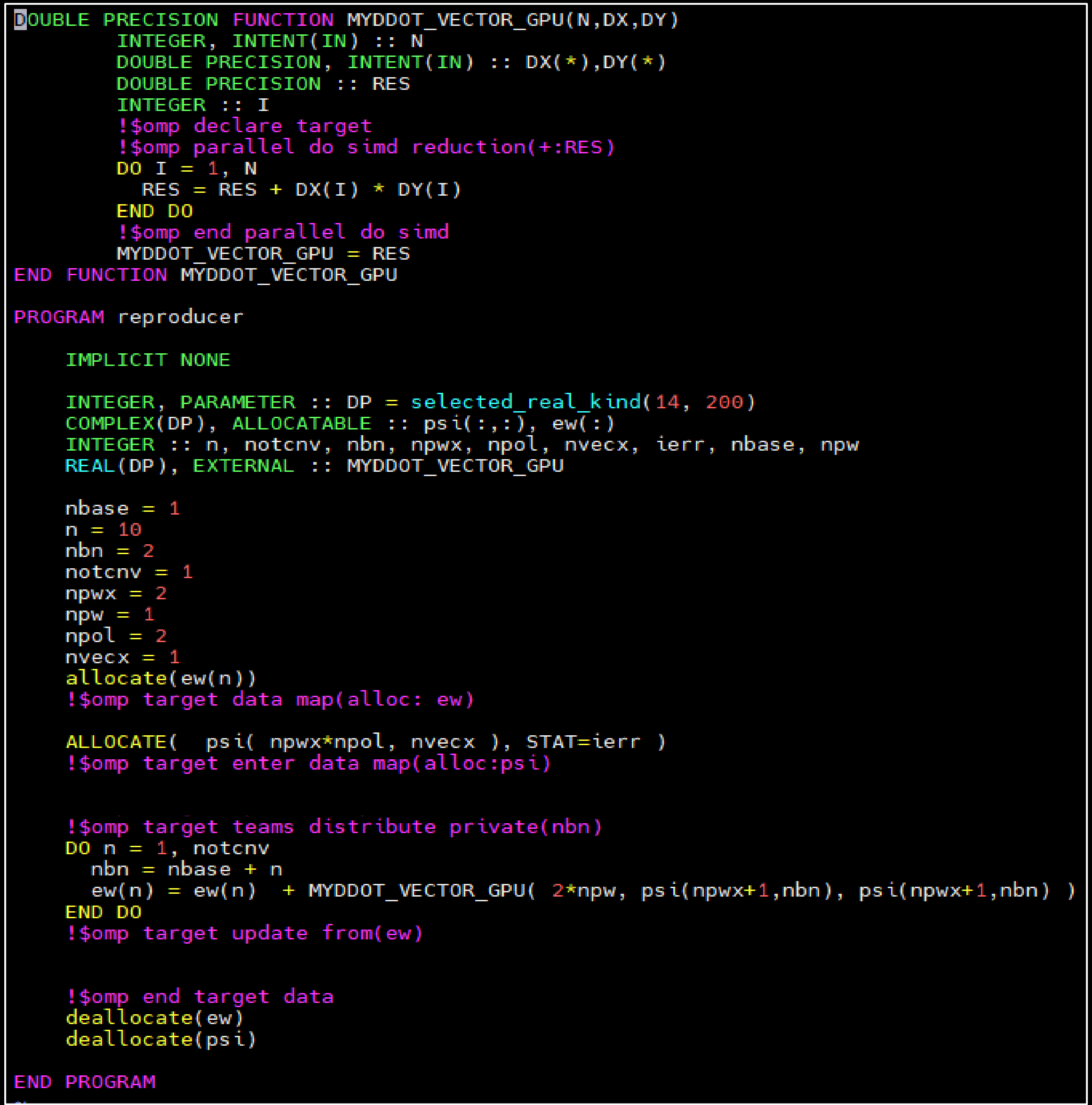


```fortran
DOUBLE PRECISION FUNCTION MYDDOT_VECTOR_GPU(N,DX,DY)
        INTEGER, INTENT(IN) :: N
        DOUBLE PRECISION, INTENT(IN) :: DX(*),DY(*)
        DOUBLE PRECISION :: RES
        INTEGER :: I
        !$omp declare target
        !$omp parallel do simd reduction(+:RES)
        DO I = 1, N
          RES = RES + DX(I) * DY(I)
        END DO
        !$omp end parallel do simd
        MYDDOT_VECTOR_GPU = RES
END FUNCTION MYDDOT_VECTOR_GPU
```



```
$make
ftn -fopenmp -c myddot.f90 -o myddot.o

        !$omp parallel do simd reduction(+:RES)
ftn-7212 ftn: WARNING MYDDOT_VECTOR_GPU, File = myddot.f90, Line = 7
  Variable "res" is used before it is defined.
ftn-7256 ftn: WARNING MYDDOT_VECTOR_GPU, File = myddot.f90, Line = 7
   An OpenMP parallel construct in a target region is limited to a single thread.

Cray Fortran : Version 15.0.0.3 (20220920162820_088e5928c3724749216ddb6b2fbbcd2152ed2bb8)
Cray Fortran : Thu Jan 05, 2023  15:58:21
Cray Fortran : Compile time:  0.0472 seconds
Cray Fortran : 13 source lines
Cray Fortran : 0 errors, 2 warnings, 0 other messages, 0 ansi
Cray Fortran : "explain ftn-message number" gives more information about each message.
ftn -fopenmp -c reproducer.f90 -o reproducer.o
ftn -fopenmp myddot.o reproducer.o -o reproducer.x
error: reproducer.f90:28:0: in function reproducer_$ck_L25_1 void (i64, i64, i64, i64, i64, i64): unsupported call
to variadic function myddot_vector_gpu_

make: *** [Makefile:8: reproducer] Error 1
```

Declare target (alternative method)



```
DOUBLE PRECISION FUNCTION MYDDOT_VECTOR_GPU(N,DX,DY)
        INTEGER, INTENT(IN) :: N
        DOUBLE PRECISION, INTENT(IN) :: DX(*),DY(*)
        DOUBLE PRECISION :: RES
        INTEGER :: I
        !$omp declare target
        !$omp parallel do simd reduction(+:RES)
        DO I = 1, N
          RES = RES + DX(I) * DY(I)
        END DO
        !$omp end parallel do simd
        MYDDOT_VECTOR_GPU = RES
END FUNCTION MYDDOT_VECTOR_GPU

PROGRAM reproducer

    IMPLICIT NONE

    INTEGER, PARAMETER :: DP = selected_real_kind(14, 200)
    COMPLEX(DP), ALLOCATABLE :: psi(:,:), ew(:)
    INTEGER :: n, notcnv, nbn, npwx, npol, nvecx, ierr, nbase, npw
    REAL(DP), EXTERNAL :: MYDDOT_VECTOR_GPU

    nbase = 1
    n = 10
    nbn = 2
    notcnv = 1
    npwx = 2
    npw = 1
    npol = 2
    nvecx = 1
    allocate(ew(n))
    !$omp target data map(alloc: ew)

    ALLOCATE(  psi( npwx*npol, nvecx ), STAT=ierr )
    !$omp target enter data map(alloc:psi)


    !$omp target teams distribute private(nbn)
    DO n = 1, notcnv
      nbn = nbase + n
      ew(n) = ew(n)  + MYDDOT_VECTOR_GPU( 2*npw, psi(npwx+1,nbn), psi(npwx+1,nbn) )
    END DO
    !$omp target update from(ew)


    !$omp end target data
    deallocate(ew)
    deallocate(psi)

END PROGRAM
```

- To get around the error, we can define function in the same file as function call
  - It would be challenging to apply his workaround in the applications with many function/subroutine calls

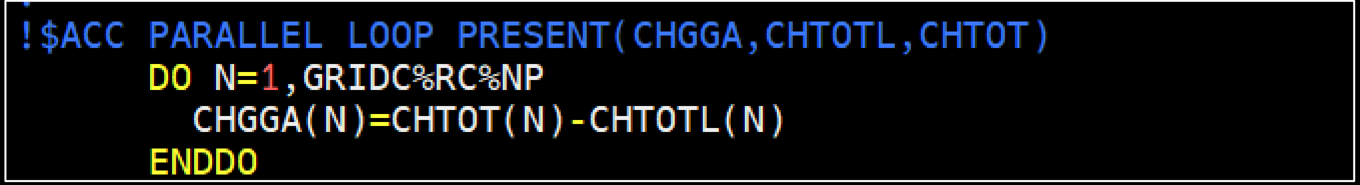
AMD
together we advance_

Content

- Introduction
- Debugging and profiling OpenMP offloading code in VASP
- OpenMP Offloading Challenges in VASP
  - Concurrent support for different directive-based paradigms
  - Enable/disable offloading in different code paths
  - Interface OMP offloading with ROCM libraries
- Compiler related challenges
  - Pointer aliasing
  - Pointer mismatch in subroutine calls
  - Atomic update
  - Declare target
- **Data management**
- Summary

Data management

- Data management is challenging in porting big applications like VASP
- The present clause in OpenACC is very helpful for data management in VASP
- In OpenMP offloading, omp_target_is_present can be used but it makes the code unmaintainable
- Present clause in OpenMP would be very useful for debugging and performance optimization



```
!$ACC PARALLEL LOOP PRESENT(CHGGA,CHTOTL,CHTOT)
      DO N=1,GRIDC%RC%NP
        CHGGA(N)=CHTOT(N)-CHTOTL(N)
      ENDDO
```

Summary

- Debugging and profiling OpenMP offloading code on AMD GPUs
- Discussed the challenges in adding OpenMP offloading support in VASP
- Compiler related challenges
  - Having a standard benchmark for capturing the compiler related issues would be helpful
- Data management
  - Having present clause in OMP offloading would be helpful to better deal with data management in big applications

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