Mixed-Language Programming with Fortran and Data Parallel C++

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Goals

- Offload computationally intensive tasks in existing Fortran code using DPC++
- Use as much of the existing Fortran code as possible and use DPC++ only for offload
- Minimize changes to the code
- Establish BKMs, patterns and designs useful for DPC++ code migration
- Quantify and compare performance (DPC++, OMP)

Code Analysis – The Driver

Bottleneck → Offload

```fortran
  call write_state_stats("Input State", log_file_unit)

  ! Get the start time
  call system_clock(count_start, count_rate)

#ifdef ENABLE_GPTL
  if (do_profile == 1) then
     ret = gptlstart('kernel')
  end if
#endif

  ! Run the kernel
  !$OMP parallel do schedule(runtime)
  do k=1, npz
     call c_sw(sw_corner, se_corner, nw_corner, ne_corner,              &
               rarea, rarea_c, sin_sg, cos_sg, sina_v, cosa_v,           &
               sina_u, cosa_u, fC, rdxc, rdyc, dx, dy, dxc, dyc,        &
               cosa_s, rsin_u, rsin_v, rsin2, dxa, dya,                 &
               delpc(isd,jsd,k), delp(isd,jsd,k), ptc(isd,jsd,k),       &
               pt(isd,jsd,k), u(isd,jsd,k), v(isd,jsd,k),               &
               w(isd,jsd,k), uc(isd,jsd,k), vc(isd,jsd,k),              &
               ua(isd,jsd,k), va(isd,jsd,k), wc(isd,jsd,k),             &
               ut(isd,jsd,k), vt(isd,jsd,k), divg_d(isd,jsd,k), dt2)
  enddo

#ifdef ENABLE_GPTL
  if (do_profile == 1) then
     ret = gptlstop('kernel')
  end if
#endif

  ! Get the stop time
  call system_clock(count_end, count_rate)

  ! Write the output state statistics to the log file
  call write_state_stats("Output State", log_file_unit)
```

Driver – in Fortran

```fortran

  !------------------------------------------------------------------
  ! c_sw
  !
  ! Top-level routine for c_sw kernel
  !------------------------------------------------------------------
  subroutine c_sw(sw_corner, se_corner, nw_corner, ne_corner,       &
                  rarea, rarea_c, sin_sg, cos_sg, sina_v, cosa_v,   &
                  sina_u, cosa_u, fC, rdxc, rdyc, dx, dy, dxc, dyc, &
                  cosa_s, rsin_u, rsin_v, rsin2, dxa, dya, delpc,   &
                  delp, ptc, pt, u, v, w, uc, vc, ua, va, wc, ut,   &
                  vt, divg_d, dt2)

    logical, intent(   in) :: sw_corner, se_corner, ne_corner, nw_corner
    real,    intent(   in), dimension(isd:ied,  jsd:jed    ) :: rarea
    real,    intent(   in), dimension(isd:ied+1,jsd:jed+1  ) :: rarea_c
    real,    intent(   in), dimension(isd:ied,  jsd:jed,  9) :: sin_sg, cos_sg
    real,    intent(   in), dimension(isd:ied,  jsd:jed+1  ) :: sina_v, cosa_v
    real,    intent(   in), dimension(isd:ied+1,jsd:jed    ) :: sina_u, cosa_u
    real,    intent(   in), dimension(isd:ied+1,jsd:jed+1  ) :: fC
    real,    intent(   in), dimension(isd:ied+1,jsd:jed    ) :: rdxc, dy, dxc
    real,    intent(   in), dimension(isd:ied,  jsd:jed+1  ) :: rdyc, dx, dyc
    real,    intent(   in), dimension(isd:ied,  jsd:jed    ) :: cosa_s
    real,    intent(   in), dimension(isd:ied+1,jsd:jed    ) :: rsin_u
    real,    intent(   in), dimension(isd:ied,  jsd:jed+1  ) :: rsin_v
    real,    intent(   in), dimension(isd:ied,  jsd:jed    ) :: rsin2, dxa, dya
    real,    intent(inout), dimension(isd:ied,  jsd:jed+1  ) :: u, vc
    real,    intent(inout), dimension(isd:ied+1,jsd:jed    ) :: v, uc
    real,    intent(inout), dimension(isd:ied,  jsd:jed    ) :: delp, pt, ua
    real,    intent(inout), dimension(isd:ied,  jsd:jed    ) :: va, ut, vt, w
    real,    intent(  out), dimension(isd:ied,  jsd:jed    ) :: delpc, ptc, wc
    real,    intent(  out), dimension(isd:ied+1,jsd:jed+ 1 ) :: divg_d
    real,    intent(   in)                                   :: dt2

    ! Local:
    real, dimension(is-1:ie+1, js-1:je+1) :: vort, ke
    real, dimension(is-1:ie+2, js-1:je+1) :: fx, fx1, fx2
    real, dimension(is-1:ie+1, js-1:je+2) :: fy, fy1, fy2
    real                                  :: dt4
    integer                               :: i, j
    integer                               :: iep1, jep1
    integer                               :: ret
```

Kernel Parameters: 2- and 3-dimensional arrays

Code Analysis – Kernel c_sw

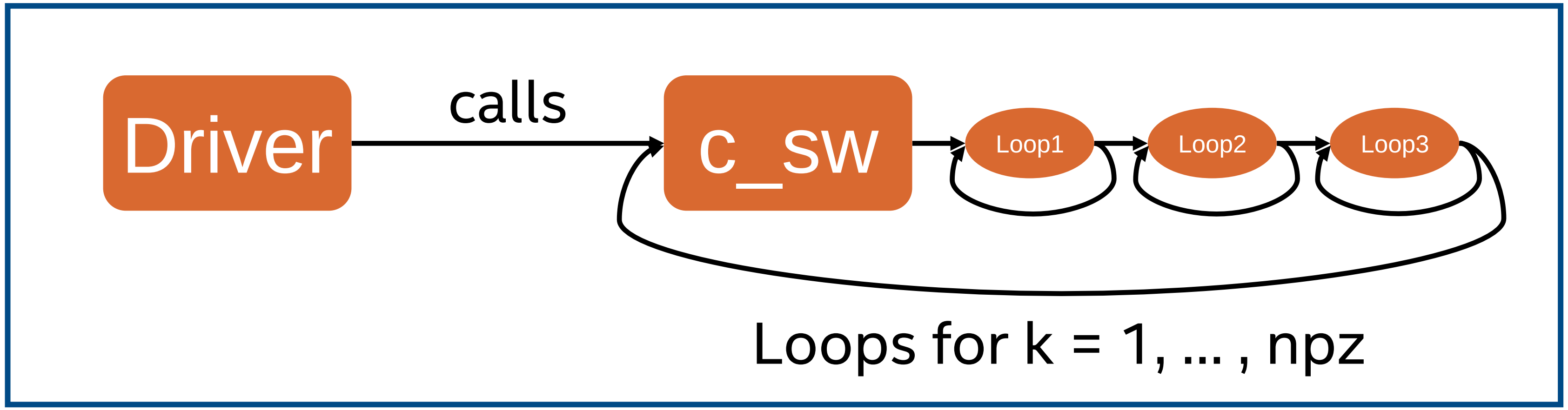
- Kernel consists of **function calls** and nested **loops**
- ~800 lines of c_sw kernel Fortran code

```fortran

    iep1 = ie + 1
    jep1 = je + 1

    call d2a2c_vect(sw_corner, se_corner, ne_corner, nw_corner,           &
                    sin_sg, cosa_u, cosa_v, cosa_s, rsin_u, rsin_v, rsin2, &
                    dxa, dya, u, v, ua, va, uc, vc, ut, vt)

    if ( nord > 0 ) then
      call divergence_corner(sw_corner, se_corner, ne_corner, nw_corner, &
                             rarea_c, sin_sg, cos_sg,                    &
                             dxc, dyc, u, v, ua, va, divg_d)
    endif

    do j = js-1, jep1
      do i = is-1, iep1+1
        if (ut(i, j) > 0.) then
              ut(i, j) = dt2 * ut(i, j) * dy(i, j) * sin_sg(i-1, j, 3)
        else
              ut(i, j) = dt2 * ut(i, j) * dy(i, j) * sin_sg(i, j, 1)
        end if
      enddo
    enddo
    do j = js-1, je+2
      do i = is-1, iep1
        if (vt(i, j) > 0.) then
          vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j-1, 4)
        else
          vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j, 2)
          end if
      enddo
    enddo

```

Piece of the kernel code

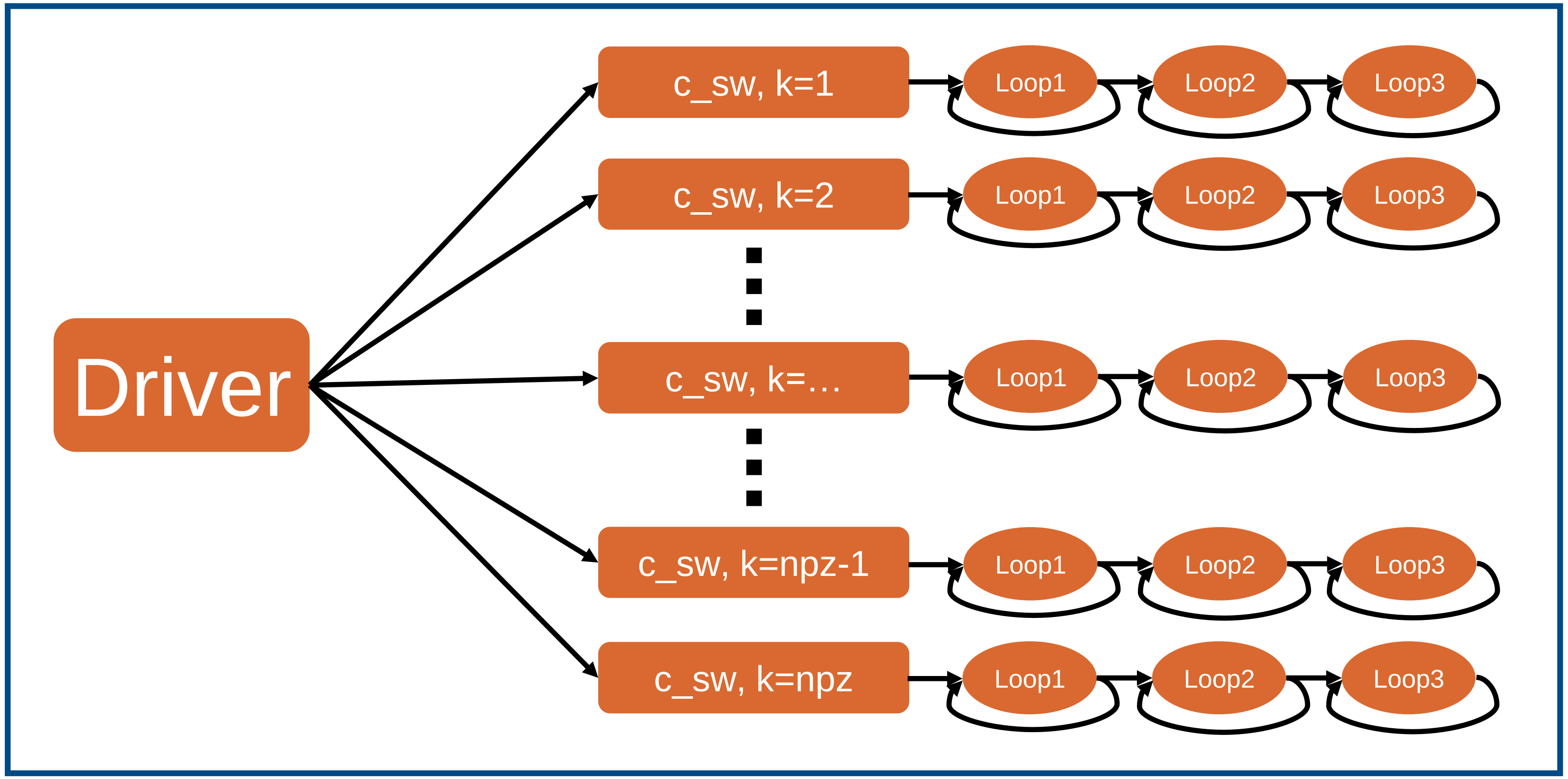
Code Flow Chart

Serial

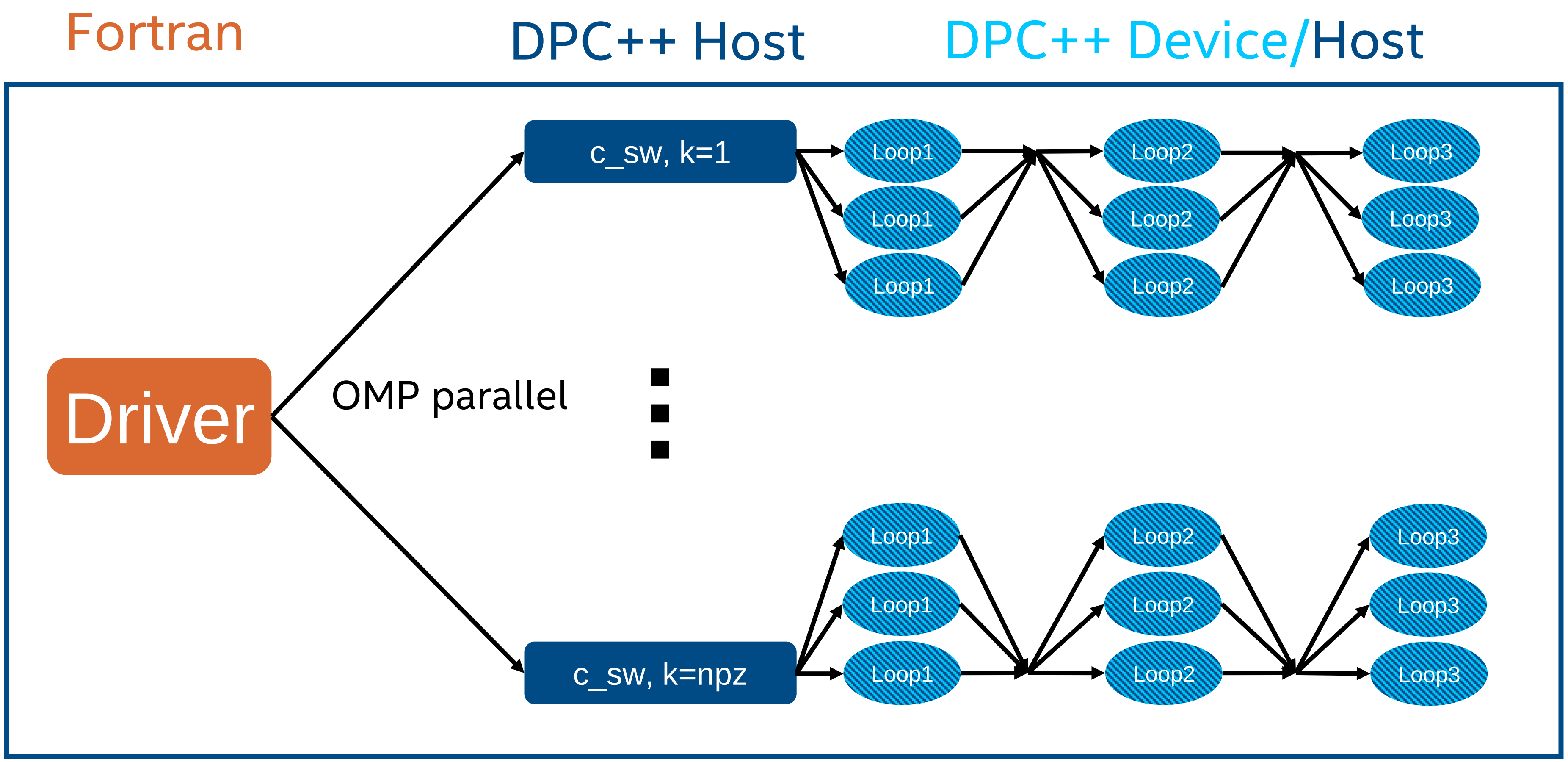


Code Flow Chart

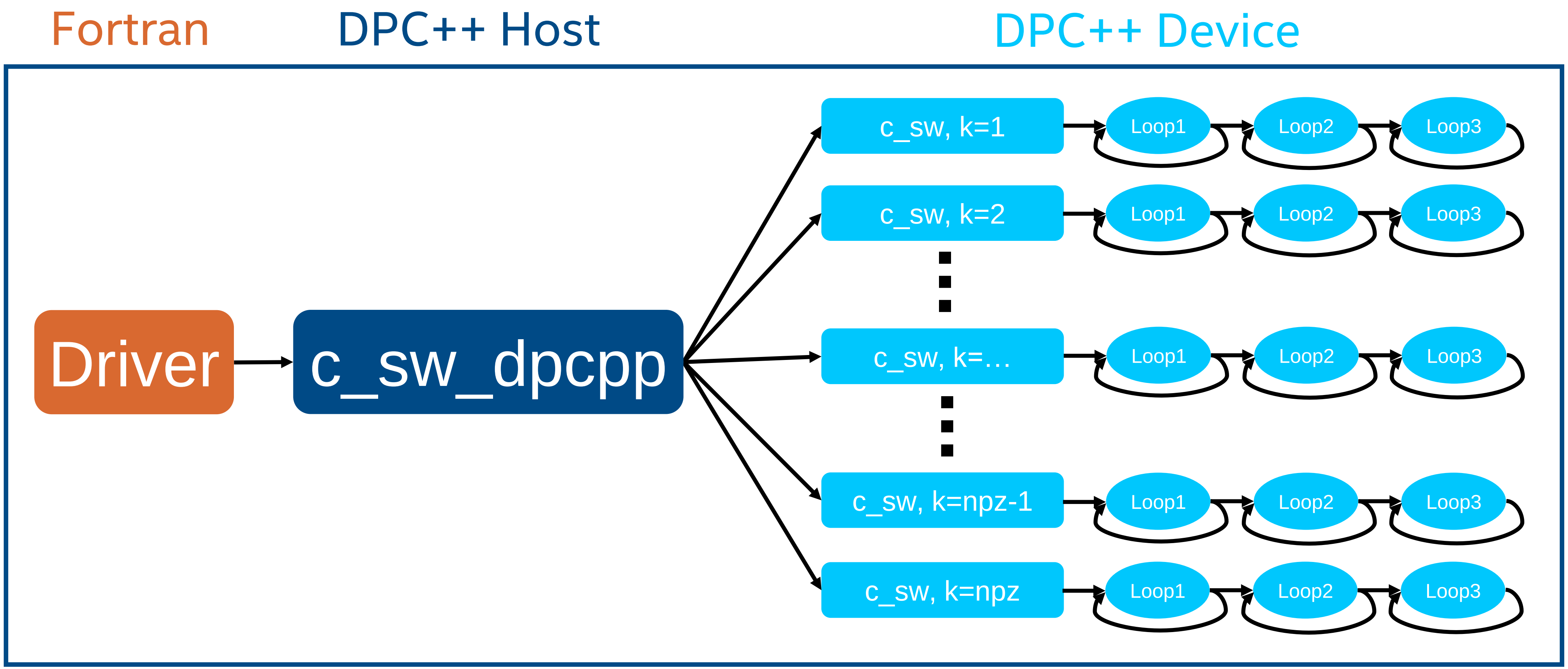
OMP parallel



Possible Offload - Approach ‘Loop’



Possible Offload - Approach ‘Outer’



Design Challenges

- Non-zero start of Fortran arrays
- Non-zero start of loops
- Fortran column-major vs C++ row-major
- Access operator in Fortran differs from C++
- No memory allocations in device code
- Many arrays as parameters
- Solution: Two step migration to C++ and then DPC++, use Approach 'Outer'

```fortran

  !-------------------------------------------------------------------
  ! c_sw
  !
  ! Top-level routine for c_sw kernel
  !-------------------------------------------------------------------
  subroutine c_sw(sw_corner, se_corner, nw_corner, ne_corner,       &
                  rarea, rarea_c, sin_sg, cos_sg, sina_v, cosa_v,   &
                  sina_u, cosa_u, fC, rdxc, rdyc, dx, dy, dxc, dyc, &
                  cosa_s, rsin_u, rsin_v, rsin2, dxa, dya, delpc,   &
                  delp, ptc, pt, u, v, w, uc, vc, ua, va, wc, ut,   &
                  vt, divg_d, dt2)

    logical, intent(   in) :: sw_corner, se_corner, ne_corner, nw_corner
    real,    intent(   in), dimension(isd:ied,   jsd:jed     ) :: rarea
    real,    intent(   in), dimension(isd:ied+1,jsd:jed+1  ) :: rarea_c
    real,    intent(   in), dimension(isd:ied,   jsd:jed,  9) :: sin_sg, cos_sg
    real,    intent(   in), dimension(isd:ied,   jsd:jed+1  ) :: sina_v, cosa_v
    real,    intent(   in), dimension(isd:ied+1,jsd:jed     ) :: sina_u, cosa_u
    real,    intent(   in), dimension(isd:ied+1,jsd:jed+1  ) :: fC
    real,    intent(   in), dimension(isd:ied+1,jsd:jed     ) :: rdxc, dy, dxc
    real,    intent(   in), dimension(isd:ied,   jsd:jed+1  ) :: rdyc, dx, dyc
    real,    intent(   in), dimension(isd:ied,   jsd:jed     ) :: cosa_s
    real,    intent(   in), dimension(isd:ied+1,jsd:jed     ) :: rsin_u
    real,    intent(   in), dimension(isd:ied,   jsd:jed+1  ) :: rsin_v
    real,    intent(   in), dimension(isd:ied,   jsd:jed     ) :: rsin2, dxa, dya
    real,    intent(inout), dimension(isd:ied,   jsd:jed+1  ) :: u, vc
    real,    intent(inout), dimension(isd:ied+1,jsd:jed     ) :: v, uc
    real,    intent(inout), dimension(isd:ied,   jsd:jed     ) :: delp, pt, ua
    real,    intent(inout), dimension(isd:ied,   jsd:jed     ) :: va, ut, vt, w
    real,    intent(  out), dimension(isd:ied,   jsd:jed     ) :: delpc, ptc, wc
    real,    intent(  out), dimension(isd:ied+1,jsd:jed+ 1 ) :: divg_d
    real,    intent(   in)                                    :: dt2

    ! Local:
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    real, dimension(is-1:ie+2, js-1:je+1) :: fx, fx1, fx2
    real, dimension(is-1:ie+1, js-1:je+2) :: fy, fy1, fy2
    real                                  :: dt4
    integer                               :: i, j
    integer                               :: iep1, jep1
    integer                               :: ret
```

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c_sw code

```fortran
    iep1 = ie + 1
    jep1 = je + 1

    call d2a2c_vect(sw_corner, se_corner, ne_corner, nw_corner,          &
                    sin_sg, cosa_u, cosa_v, cosa_s, rsin_u, rsin_v, rsin2, &
                    dxa, dya, u, v, ua, va, uc, vc, ut, vt)

    if ( nord > 0 ) then
      call divergence_corner(sw_corner, se_corner, ne_corner, nw_corner, &
                             rarea_c, sin_sg, cos_sg,                    &
                             dxc, dyc, u, v, ua, va, divg_d)
    endif

    do j = js-1, jep1
      do i = is-1, iep1+1
        if (ut(i, j) > 0.) then
              ut(i, j) = dt2 * ut(i, j) * dy(i, j) * sin_sg(i-1, j, 3)
        else
              ut(i, j) = dt2 * ut(i, j) * dy(i, j) * sin_sg(i, j, 1)
        end if
      enddo
    enddo
    do j = js-1, je+2
      do i = is-1, iep1
        if (vt(i, j) > 0.) then
          vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j-1, 4)
        else
          vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j, 2)
          end if
      enddo
    enddo
```

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                    sin_sg, cosa_u, cosa_v, cosa_s, rsin_u, rsin_v, rsin2, &
                    dxa, dya, u, v, ua, va, uc, vc, ut, vt)

    if ( nord > 0 ) then
      call divergence_corner(sw_corner, se_corner, ne_corner, nw_corner, &
                             rarea_c, sin_sg, cos_sg,                    &
                             dxc, dyc, u, v, ua, va, divg_d)
    endif

    do j = js-1, jep1
      do i = is-1, iep1+1
        if (ut(i, j) > 0.) then
              ut(i, j) = dt2 * ut(i, j) * dy(i, j) * sin_sg(i-1, j, 3)
        else
              ut(i, j) = dt2 * ut(i, j) * dy(i, j) * sin_sg(i, j, 1)
        end if
      enddo
    enddo
    do j = js-1, je+2
      do i = is-1, iep1
        if (vt(i, j) > 0.) then
          vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j-1, 4)
        else
          vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j, 2)
          end if
      enddo
    enddo

```

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iep1 = ie + 1
jep1 = je + 1

call d2a2c_vect(sw_corner, se_corner, ne_corner, nw_corner,            &
                sin_sg, cosa_u, cosa_v, cosa_s, rsin_u, rsin_v, rsin2, &
                dxa, dya, u, v, ua, va, uc, vc, ut, vt)

if ( nord > 0 ) then
  call divergence_corner(sw_corner, se_corner, ne_corner, nw_corner, &
                         rarea_c, sin_sg, cos_sg,                    &
                         dxc, dyc, u, v, ua, va, divg_d)
endif

do j = js-1, jep1
  do i = is-1, iep1+1
    if (ut(i, j) > 0.) then
       ut(i, j) = dt2 * ut(i, j) * dy(i, j) * sin_sg(i-1, j, 3)
    else
       ut(i, j) = dt2 * ut(i, j) * dy(i, j) * sin_sg(i, j, 1)
    end if
  enddo
enddo
do j = js-1, je+2
  do i = is-1, iep1
    if (vt(i, j) > 0.) then
      vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j-1, 4)
    else
      vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j, 2)
    end if
  enddo
enddo
```

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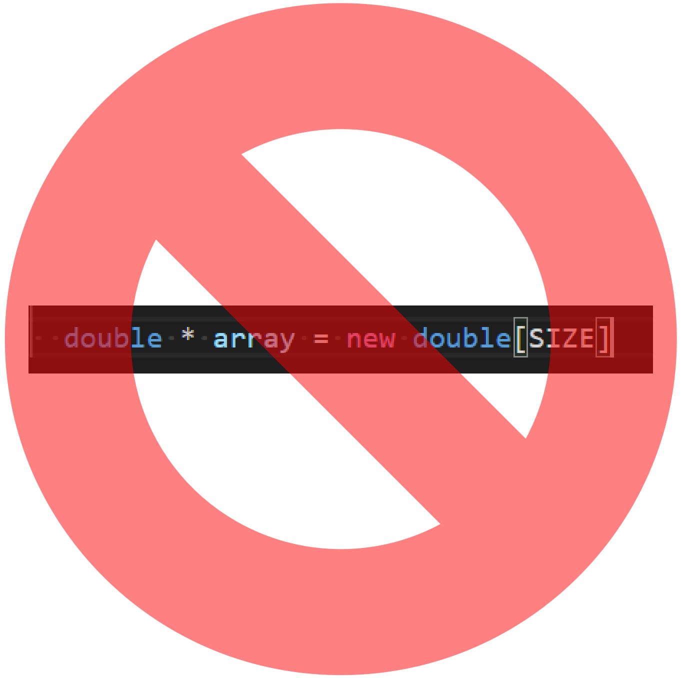

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- Solution: Two step migration to C++ and then DPC++, use Approach ‘Outer’

```
  call write_state_stats("Input State", log_file_unit)

  ! Get the start time
  call system_clock(count_start, count_rate)

#ifdef ENABLE_GPTL
  if (do_profile == 1) then
    ret = gptlstart('kernel')
  end if
#endif

  ! Run the kernel
  !$OMP parallel do schedule(runtime)
  do k=1, npz
    call c_sw(sw_corner, se_corner, nw_corner, ne_corner,                  &
              rarea, rarea_c, sin_sg, cos_sg, sina_v, cosa_v,              &
              sina_u, cosa_u, fC, rdxc, rdyc, dx, dy, dxc, dyc,            &
              cosa_s, rsin_u, rsin_v, rsin2, dxa, dya,                     &
              delpc(isd,jsd,k), delp(isd,jsd,k), ptc(isd,jsd,k),           &
              pt(isd,jsd,k), u(isd,jsd,k), v(isd,jsd,k),                   &
              w(isd,jsd,k), uc(isd,jsd,k), vc(isd,jsd,k),                  &
              ua(isd,jsd,k), va(isd,jsd,k), wc(isd,jsd,k),                 &
              ut(isd,jsd,k), vt(isd,jsd,k), divg_d(isd,jsd,k), dt2)
  enddo

#ifdef ENABLE_GPTL
  if (do_profile == 1) then
    ret = gptlstop('kernel')
  end if
#endif

  ! Get the stop time
  call system_clock(count_end, count_rate)

  ! Write the output state statistics to the log file
  call write_state_stats("Output State", log_file_unit)
```

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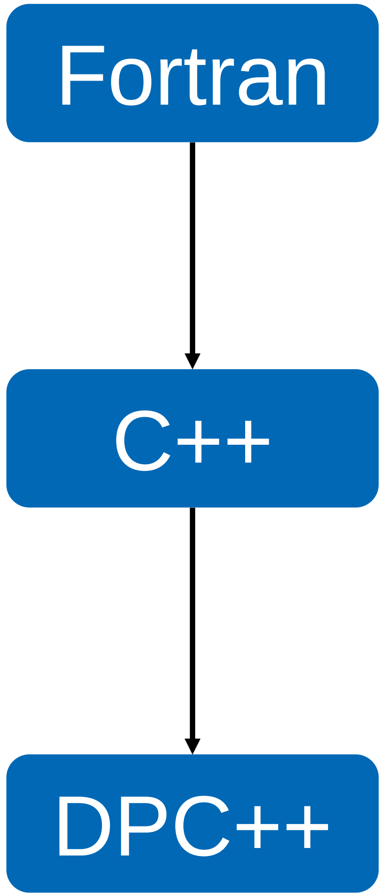

Challenges Fortran - C++

- Main Issue: Array Indexing
  - Unit stride is inner index in Fortran vs outer in C++
  - Non-zero indexing in Fortran possible (and used in code)

- Solution: Class OffsetArray (1D, 2D, 3D) wrapping dynamic array emulating Fortran style arrays (see Figure)

```cpp
template <class T>
class OffsetArray
{
    const int istart;
    const int iend;
    T * const values;

  public:

    OffsetArray(int istart_in, int iend_in) :
      istart(std::min(istart_in, iend_in)),
      iend(std::max(istart_in, iend_in)),
      values(new T[iend-istart+1])
    {
    }

    ~OffsetArray() {
        delete [] values;
    }

    T &operator() (int i) {
      const int index=i-istart;
      return values[index];
    }

};


/////USAGE/////
int main()
{
    OffsetArray<double> u(5, 10);
    u(5) = 1.0;
}
```

Fortran - C++ Code Comparison

Fortran

```fortran
call d2a2c_vect(sw_corner, se_corner, ne_corner, nw_corner,            &
                sin_sg, cosa_u, cosa_v, cosa_s, rsin_u, rsin_v, rsin2, &
                dxa, dya, u, v, ua, va, uc, vc, ut, vt)

if ( nord > 0 ) then
  call divergence_corner(sw_corner, se_corner, ne_corner, nw_corner, &
                         rarea_c, sin_sg, cos_sg,                    &
                         dxc, dyc, u, v, ua, va, divg_d)
endif

do j = js-1, jep1
  do i = is-1, iep1+1
    if (ut(i, j) > 0.) then
          ut(i, j) = dt2 * ut(i, j) * dy(i, j) * sin_sg(i-1, j, 3)
    else
          ut(i, j) = dt2 * ut(i, j) * dy(i, j) * sin_sg(i, j, 1)
    end if
  enddo
enddo
do j = js-1, je+2
  do i = is-1, iep1
    if (vt(i, j) > 0.) then
      vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j-1, 4)
    else
      vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j, 2)
      end if
  enddo
enddo
```

C++

```cpp
d2a2c_vect(sw_corner, se_corner, ne_corner, nw_corner, sin_sg, cosa_u,
    cosa_v, cosa_s, rsin_u, rsin_v, rsin2, dxa, dya, u, v, ua, va, uc, vc,
    ut, vt);

if (nord > 0)
{
  divergence_corner(sw_corner, se_corner, ne_corner, nw_corner,
                    rarea_c, sin_sg, cos_sg, dxc, dyc, u, v, ua, va, divg_d);
}

for (j=js-1; j<=jep1; j++)
{
  for (i=is-1; i<=iep1+1; i++)
  {
    if (ut(i,j)>0.0)
      ut(i,j)=dt2*ut(i,j)*dy(i,j)*sin_sg(i-1,j,3);
    else
      ut(i,j)=dt2*ut(i,j)*dy(i,j)*sin_sg(i,j,1);
  }
}

for (j=js-1; j<=je+2; j++)
{
  for (i=is-1; i<=iep1; i++)
  {
    if (vt(i,j)>0.0)
      vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j-1, 4);
    else
      vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j, 2);
  }
}
```

Challenges C++ - DPC++

- Main Issues:
  - OffsetArray class cannot be used in device code (as it is)
  - DPC++ parallel_for indices start at 0 (‘loop indexing starting at 0’)

- Solutions:
  - Naively: Simple offsets based on loop and array start index
  - Better: Adjusting the OffsetArray class and use Approach ‘Outer’

C++ - DPC++ Code Comparison: Naively

C++

```cpp
d2a2c_vect(sw_corner, se_corner, ne_corner, nw_corner, sin_sg, cosa_u,
        cosa_v, cosa_s, rsin_u, rsin_v, rsin2, dxa, dya, u, v, ua, va, uc, vc,
        ut, vt);

if (nord > 0)
{
  divergence_corner(sw_corner, se_corner, ne_corner, nw_corner,
                    rarea_c, sin_sg, cos_sg, dxc, dyc, u, v, ua, va, divg_d);
}

for (j=js-1; j<=jep1; j++)
{
  for (i=is-1; i<=iep1+1; i++)
  {
    if (ut(i,j)>0.0)
      ut(i,j)=dt2*ut(i,j)*dy(i,j)*sin_sg(i-1,j,3);
    else
      ut(i,j)=dt2*ut(i,j)*dy(i,j)*sin_sg(i,j,1);
  }
}

for (j=js-1; j<=je+2; j++)
{
  for (i=is-1; i<=iep1; i++)
  {
    if (vt(i,j)>0.0)
      vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j-1, 4);
    else
      vt(i, j) = dt2 * vt(i, j) * dx(i, j) * sin_sg(i, j, 2);
  }
}
```

DPC++

```cpp
d2a2c_vect();

if (nord > 0)
  divergence_corner();


Q_.submit([&](handler &h) {
  accessor abut{but, h, read_write};
  accessor abdy{bdy, h, read_only};
  accessor absin_sg{bsin_sg, h, read_only};
  const int i_off = -isd + is-1;
  const int j_off = -jsd + js-1;
  const int k_off = -1;
  h.parallel_for(range<2>{static_cast<size_t>(jep1-(js-1)+1), static_cast<size_t>(iep1+1-(is-1)+1)}, [=](id<2> idx) {
    const int i = idx[1] + i_off;
    const int j = idx[0] + j_off;
    if (abut[j][i]>0.0)
      abut[j][i]=ldt2*abut[j][i]*abdy[j][i]*absin_sg[3+k_off][j][i-1];
    else
      abut[j][i]=ldt2*abut[j][i]*abdy[j][i]*absin_sg[1+k_off][j][i];
  });
});

Q_.submit([&](handler &h) {
  accessor abvt{bvt, h, read_write};
  accessor abdx{bdx, h, read_only};
  accessor absin_sg{bsin_sg, h, read_only};
  const int i_off = -isd + is-1;
  const int j_off = -jsd + js-1;
  const int k_off = -1;
  h.parallel_for(range<2>{static_cast<size_t>(je+2-(js-1)+1), static_cast<size_t>(iep1-(is-1)+1)}, [=](id<2> idx) {
    const int i = idx[1] + i_off;
    const int j = idx[0] + j_off;
    if (abvt[j][i]>0.0)
      abvt[j][i]=ldt2*abvt[j][i]*abdx[j][i]*absin_sg[4+k_off][j-1][i];
    else
      abvt[j][i]=ldt2*abvt[j][i]*abdx[j][i]*absin_sg[2+k_off][j][i];
  });
});
```

} DPC++ Accessors

} Offsets due to array and loop

For loop range

C++ - DPC++ Code Comparison: Naively

- Tedious migration
- Hard-to-read code
- Need to rewrite everything carefully
- Debugging is a horror
- Focus on Approach 'Outer'

Adjusting OffsetArray

- Challenges when implicitly copying objects from host to device
  - Trivial destructor required
  - Const access operator necessary (copy to device is by const value)
  - No memory allocations in device code possible; Host needs to handle memory

```cpp
template <class T>
class OffsetArray
{
    const int istart;
    const int iend;
    T * const values;

  public:
    OffsetArray() = delete;

    OffsetArray(int istart_in, int iend_in, T * values_in) :
      istart(istart_in),
      iend(istart_in),
      values(values_in)
    {
    }

    T &operator()(int i) const
    {
      return values[i-istart];
    }
};
```

Adjusting OffsetArray

- Challenges when implicitly copying objects from host to device
  - Trivial destructor required
  - Const access operator necessary (copy to device is by const value)
  - No memory allocations in device code possible; Host needs to handle memory

```
template <class T>
class OffsetArray
{
    const int istart;
    const int iend;
    T * const values;

  public:
    OffsetArray() = delete;

    OffsetArray(int istart_in, int iend_in, T * values_in) :
        istart(istart_in),
        iend(istart_in),
        values(values_in)
    {
    }

    T &operator()(int i) const
    {
        return values[i-istart];
    }
};
```

Adjusting the OffsetArray Class for Approach 2

- Challenges when implicitly copying objects from host to device
  - Trivial destructor required
  - Const access operator necessary (copy to device is by const value)
  - No memory allocations in device code possible; Host needs to handle memory

```cpp
template <class T>
class OffsetArray
{
    const int istart;
    const int iend;
    T * const values;

  public:
    OffsetArray() = delete;

    OffsetArray(int istart_in, int iend_in, T * values_in) :
        istart(istart_in),
        iend(istart_in),
        values(values_in)
    {
    }

    T &operator()(int i) const
    {
        return values[i-istart];
    }
};
```

Usage of the OffsetArray

- Allocate device memory explicitly
- Construct OffsetArray with it
- Copy memory back to host after device code execution
- Free device memory explicitly after device code execution
- Minimize allocations and copies between host and device
- OffsetArray can be used on host and device

```cpp
template <class T>
class OffsetArray
{
    const int istart;
    const int iend;
    T * const values;

  public:
    OffsetArray() = delete;

    OffsetArray(int istart_in, int iend_in, T * values_in) :
        istart(istart_in),
        iend(istart_in),
        values(values_in)
    {
    }

    T &operator()(int i) const
    {
        return values[i-istart];
    }
};
```

Variations of the OffsetArray

- Can use accessors to buffers instead of USM (T * const)
- Shared memory (malloc_shared) is also a possibility → can be used on host and device with implicit copying → would work well for Approach ‘Loop’
- A possible extension would be a factory pattern for the generation of the OffsetArray

```cpp
template <class T>
class OffsetArray
{
    const int istart;
    const int iend;
    T * const values;

  public:
    OffsetArray() = delete;

    OffsetArray(int istart_in, int iend_in, T * values_in) :
        istart(istart_in),
        iend(istart_in),
        values(values_in)
    {
    }

    T &operator()(int i) const
    {
        return values[i-istart];
    }
};
```

Putting Everything Together

Fortran Driver

```fortran
! Run the kernel
call c_sw_dpcpp(isd, ied, jsd, jed, is, ie, js, je, nord, npx, npy,  &
                npz, do_profile, dt2,                                &
                sw_corner, se_corner, nw_corner, ne_corner,          &
                rarea, rarea_c, sin_sg, cos_sg, sina_v, cosa_v,      &
                sina_u, cosa_u, fC, rdxc, rdyc, dx, dy, dxc, dyc,    &
                cosa_s, rsin_u, rsin_v, rsin2, dxa, dya,             &
                delpc, delp, ptc, pt, u, v, w, uc, vc, ua, va, wc,   &
                ut, vt, divg_d)

! !$OMP parallel do schedule(runtime)
! do k=1, npz
!    call c_sw(sw_corner, se_corner, nw_corner, ne_corner,    &
!              delpc(isd,jsd,k), delp(isd,jsd,k), ptc(isd,jsd,k),    &
!              pt(isd,jsd,k), u(isd,jsd,k), v(isd,jsd,k),            &
!              w(isd,jsd,k), uc(isd,jsd,k), vc(isd,jsd,k),           &
!              ua(isd,jsd,k), va(isd,jsd,k), wc(isd,jsd,k),          &
!              ut(isd,jsd,k), vt(isd,jsd,k), divg_d(isd,jsd,k), dt2)
! enddo
```

DPC++ Device Code = C++ Code

```cpp
d2a2c_vect(u, v, ua, va, uc, vc, ut, vt, utmp, vtmp);


if (nord > 0)
{
  divergence_corner(u, v, ua, va, divg_d, uf, vf);
}

for (j=js-1; j<=jep1; j++)
{
  for (i=is-1; i<=iep1+1; i++)
  {
    if (ut(i,j)>0.0)
      ut(i,j)=dt2*ut(i,j)*dy(i,j)*sin_sg(i-1,j,3);
    else
      ut(i,j)=dt2*ut(i,j)*dy(i,j)*sin_sg(i,j,1);
  }
}


for (j=js-1; j<=je+2; j++)
{
  for (i=is-1; i<=iep1; i++)
  {
    if (vt(i,j)>0.0)
      vt(i,j) = dt2 * vt(i,j) * dx(i, j) * sin_sg(i, j-1, 4);
    else
      vt(i,j) = dt2 * vt(i,j) * dx(i, j) * sin_sg(i, j, 2);
  }
}
```

Fortran Driver

```fortran

#ifdef ENABLE_GPTL
  if (do_profile == 1) then
      ret = gptlstart('kernel')
  end if
#endif

  ! Run the kernel
  call c_sw_dpcpp(isd, ied, jsd, jed, is, ie, js, je, nord, npx, npy,  &
              npz, do_profile, dt2,                                     &
              sw_corner, se_corner, nw_corner, ne_corner,               &
              rarea, rarea_c, sin_sg, cos_sg, sina_v, cosa_v,           &
              sina_u, cosa_u, fC, rdxc, rdyc, dx, dy, dxc, dyc,         &
              cosa_s, rsin_u, rsin_v, rsin2, dxa, dya,                  &
              delpc, delp, ptc, pt, u, v, w, uc, vc, ua, va, wc,        &
              ut, vt, divg_d)

  ! !$OMP parallel do schedule(runtime)
  ! do k=1, npz
  !    call c_sw(sw_corner, se_corner, nw_corner, ne_corner,    &
  !              delpc(isd,jsd,k), delp(isd,jsd,k), ptc(isd,jsd,k),    &
  !              pt(isd,jsd,k), u(isd,jsd,k), v(isd,jsd,k),            &
  !              w(isd,jsd,k), uc(isd,jsd,k), vc(isd,jsd,k),           &
  !              ua(isd,jsd,k), va(isd,jsd,k), wc(isd,jsd,k),          &
  !              ut(isd,jsd,k), vt(isd,jsd,k), divg_d(isd,jsd,k), dt2)
  ! enddo

```

→

New DPC++ c_sw_dpcpp

```cpp
Q.submit([&](handler &h) {
  CSW Foo(isd, ied, jsd, jed, is, ie, js, je, nord, npx, npy, npz, do_profile,
      dt2, sw_corner, se_corner, nw_corner, ne_corner, rarea, rarea_c, sin_sg,
      cos_sg, sina_v, cosa_v, sina_u, cosa_u, fC, rdxc, rdyc, dx, dy, dxc, dyc,
      cosa_s, rsin_u, rsin_v, rsin2, dxa, dya);

  h.parallel_for(npz, [=](auto k) {
    Offset2DArray<double, true> delpc(isd, ied, jsd, jed, pdelpc+k*isize*jsize);
    Offset2DArray<double, true> delp(isd, ied, jsd, jed, pdelp+k*isize*jsize);
    Offset2DArray<double, true> ptc(isd, ied, jsd, jed, pptc+k*isize*jsize);
    Offset2DArray<double, true> pt(isd, ied, jsd, jed, ppt+k*isize*jsize);
    Offset2DArray<double, true> u(isd, ied, jsd, jed+1, pu+k*isize*jsizep1);
    Offset2DArray<double, true> v(isd, ied+1, jsd, jed, pv+k*isizep1*jsize);
    Offset2DArray<double, true> w(isd, ied, jsd, jed, pw+k*isize*jsize);
    Offset2DArray<double, true> uc(isd, ied+1, jsd, jed, puc+k*isizep1*jsize);
    Offset2DArray<double, true> vc(isd, ied, jsd, jed+1, pvc+k*isize*jsizep1);
    Offset2DArray<double, true> ua(isd, ied, jsd, jed, pua+k*isize*jsize);
    Offset2DArray<double, true> va(isd, ied, jsd, jed, pva+k*isize*jsize);
    Offset2DArray<double, true> wc(isd, ied, jsd, jed, pwc+k*isize*jsize);
    Offset2DArray<double, true> ut(isd, ied, jsd, jed, put+k*isize*jsize);
    Offset2DArray<double, true> vt(isd, ied, jsd, jed, pvt+k*isize*jsize);
    Offset2DArray<double, true> divg_d(isd, ied+1, jsd, jed+1, pdivg_d+k*isizep1*jsizep1);

    Offset2DArray<double, true> vort(is-1, ie+1, js-1, je+1, pvort+k*bufisize*bufjsize);
    Offset2DArray<double, true> ke(is-1, ie+1, js-1, je+1, pke+k*bufisize*bufjsize);
    Offset2DArray<double, true> fx(is-1, ie+2, js-1, je+1, pfx+k*bufisizep1*bufjsize);
    Offset2DArray<double, true> fx1(is-1, ie+2, js-1, je+1, pfx1+k*bufisizep1*bufjsize);
    Offset2DArray<double, true> fx2(is-1, ie+2, js-1, je+1, pfx2+k*bufisizep1*bufjsize);
    Offset2DArray<double, true> fy(is-1, ie+1, js-1, je+2, pfy+k*bufisize*bufjsizep1);
    Offset2DArray<double, true> fy1(is-1, ie+1, js-1, je+2, pfy1+k*bufisize*bufjsizep1);
    Offset2DArray<double, true> fy2(is-1, ie+1, js-1, je+2, pfy2+k*bufisize*bufjsizep1);
    Offset2DArray<double, true> utmp(isd, ied, jsd, jed, putmp+k*isize*jsize);
    Offset2DArray<double, true> vtmp(isd, ied, jsd, jed, pvtmp+k*isize*jsize);
    Offset2DArray<double, true> uf(is-2, ie+2, js-1, je+2, puf+k*(bufisize+2)*bufjsizep1);
    Offset2DArray<double, true> vf(is-1, ie+2, js-2, je+2, pvf+k*bufisizep1*(bufjsize+2));

    Foo.c_sw(delpc, delp, ptc, pt, u, v, w, uc, vc, ua, va, wc, ut, vt, divg_d,
      vort, ke, fx, fx1, fx2, fy, fy1, fy2, utmp, vtmp, uf, vf);
  });
}).wait();

```

→

DPC++ Device Code

```cpp
d2a2c_vect(u, v, ua, va, uc, vc, ut, vt, utmp, vtmp);


if (nord > 0)
{
  divergence_corner(u, v, ua, va, divg_d, uf, vf);
}

for (j=js-1; j<=jep1; j++)
{
  for (i=is-1; i<=iep1+1; i++)
  {
    if (ut(i,j)>0.0)
      ut(i,j)=dt2*ut(i,j)*dy(i,j)*sin_sg(i-1,j,3);
    else
      ut(i,j)=dt2*ut(i,j)*dy(i,j)*sin_sg(i,j,1);
  }
}


for (j=js-1; j<=je+2; j++)
{
  for (i=is-1; i<=iep1; i++)
  {
    if (vt(i,j)>0.0)
      vt(i,j) = dt2 * vt(i,j) * dx(i, j) * sin_sg(i, j-1, 4);
    else
      vt(i,j) = dt2 * vt(i,j) * dx(i, j) * sin_sg(i, j, 2);
  }
}

```

Compilation

- export FC=ifx
- export CXX=dpcpp
- Link for_main.o
- Use linker flag –lifcore
- Use dpcpp for linking

```cmake
cmake_minimum_required( VERSION 3.10 )

project( c_sw LANGUAGES Fortran C CXX)

list( APPEND CMAKE_MODULE_PATH ${CMAKE_CURRENT_SOURCE_DIR}/cmake )
set( CMAKE_DIRECTORY_LABELS ${PROJECT_NAME} )
set( CMAKE_EXE_LINKER_FLAGS "-g -lifcore" )

enable_testing()

include(${PROJECT_NAME}_compiler_flags)

find_package( OpenMP COMPONENTS C Fortran )
find_package( NetCDF REQUIRED COMPONENTS C Fortran )

add_subdirectory(src)
add_subdirectory(test)

set_target_properties( ${PROJECT_NAME} PROPERTIES LINKER_LANGUAGE CXX )
```

CMakeLists.txt

```cmake
SET(OBJS
  /global/panfs01/admin/opt/intel/oneAPI/2021.1.2/compiler/2021.1.2/linux/compiler/lib/intel64_lin/for_main.o
)

add_executable( ${PROJECT_NAME} ${OBJS} ${c_sw_src_files} )
```

src/CMakeLists.txt

Compilation

- export FC=ifx
- export CXX=dpcpp
- Link for_main.o
- Use linker flag –lifcore
- Use dpcpp for linking

```
cmake_minimum_required( VERSION 3.10 )

project( c_sw LANGUAGES Fortran C CXX)

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CMakeLists.txt

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project( c_sw LANGUAGES Fortran C CXX)

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set( CMAKE_DIRECTORY_LABELS ${PROJECT_NAME} )
set( CMAKE_EXE_LINKER_FLAGS "-g -lifcore" )

enable_testing()

include(${PROJECT_NAME}_compiler_flags)

find_package( OpenMP COMPONENTS C Fortran )
find_package( NetCDF REQUIRED COMPONENTS C Fortran )

add_subdirectory(src)
add_subdirectory(test)

set_target_properties( ${PROJECT_NAME} PROPERTIES LINKER_LANGUAGE CXX )
```

CMakeLists.txt

```
SET(OBJS
  /global/panfs01/admin/opt/intel/oneAPI/2021.1.2/compiler/2021.1.2/linux/compiler/lib/intel64_lin/for_main.o
)

add_executable( ${PROJECT_NAME} ${OBJS} ${c_sw_src_files} )
```

src/CMakeLists.txt

Compilation

- export FC=ifx
- export CXX=dpcpp
- Link for_main.o
- Use linker flag –lifcore
- Use dpcpp for linking

```
cmake_minimum_required( VERSION 3.10 )

project( c_sw LANGUAGES Fortran C CXX)

list( APPEND CMAKE_MODULE_PATH ${CMAKE_CURRENT_SOURCE_DIR}/cmake )
set( CMAKE_DIRECTORY_LABELS ${PROJECT_NAME} )
set( CMAKE_EXE_LINKER_FLAGS "-g -lifcore" )

enable_testing()

include(${PROJECT_NAME}_compiler_flags)

find_package( OpenMP COMPONENTS C Fortran )
find_package( NetCDF REQUIRED COMPONENTS C Fortran )

add_subdirectory(src)
add_subdirectory(test)

set_target_properties( ${PROJECT_NAME} PROPERTIES LINKER_LANGUAGE CXX )
```

CMakeLists.txt

```
SET(OBJS
  /global/panfs01/admin/opt/intel/oneAPI/2021.1.2/compiler/2021.1.2/linux/compiler/lib/intel64_lin/for_main.o
)

add_executable( ${PROJECT_NAME} ${OBJS} ${c_sw_src_files} )
```

src/CMakeLists.txt

OMP Offload – Approach ‘Loop’

Fortran OMP Offload

```fortran
!$omp target parallel do private(i,j) map(to:js,je,is,ie,npy) &
!$omp map(to: va,dya,sin_sg,vtmp,u,cosa_v,rsin_v) &
!$omp map(tofrom: vt,vc)
do j = js-1, je+2
  if ( j == 1 ) then
    do i = is-1, ie+1
      vt(i, j) = edge_interpolate4(va(i, -1:2), dya(i, -1:2))
      if ( vt(i, j) < 0. ) then
        vc(i, j) = vt(i, j) * sin_sg(i, j-1, 4)
      else
        vc(i, j) = vt(i, j) * sin_sg(i, j, 2)
      end if
    enddo
  elseif ( j == 0 .or. j == (npy-1) ) then
    do i = is-1, ie+1
      vc(i, j) = c1 * vtmp(i, j-2) + c2 * vtmp(i, j-1) + c3 * vtmp(i, j)
      vt(i, j) = (vc(i, j) - u(i, j) * cosa_v(i, j)) * rsin_v(i, j)
    enddo
  elseif ( j == 2 .or. j == (npy+1) ) then
    do i = is-1, ie+1
      vc(i, j) = c1 * vtmp(i, j+1) + c2 * vtmp(i, j) + c3 * vtmp(i, j-1)
      vt(i, j) = (vc(i, j) - u(i, j) * cosa_v(i, j)) * rsin_v(i, j)
    enddo
```

DPC++ Offload

```cpp
Q.parallel_for(static_cast<size_t>((je+2)-(js-1)+1),
  [=](id<1> idx) {
  const int j = idx[0] + js-1;
  int i;

  if ( j == 1 )
  {
    for (i = is-1; i<= ie+1; i++)
    {
      //vt(i, j) = edge_interpolate4(va(i, -1:2), dya(i, -1:2))
      double va_interp[4];
      double dya_interp[4];
      for (int k=0;k<=3;k++)
      {
        va_interp[k]=va(i,k-1);
        dya_interp[k]=dya(i,k-1);
      }

      vt(i,j)=edge_interpolate4(va_interp, dya_interp);
      if ( vt(i, j) < 0. )
        vc(i, j) = vt(i, j) * sin_sg(i, j-1, 4);
      else
        vc(i, j) = vt(i, j) * sin_sg(i, j, 2);
    }
  }
```

OMP Offload – Approach ‘Outer’

Fortran OMP Offload

```fortran
  ! Run the kernel
  !$omp target map(to:sw_corner,se_corner,ne_corner,nw_corner,rarea) &
    !$omp map(to:rarea_c,sin_sg,cos_sg,sina_v,cosa_v,sina_u,cosa_u,fC) &
    !$omp map(to:rdxc,dy,dxc,rdyc,dx,dyc,cosa_s,rsin_u,rsin_v,rsin2) &
    !$omp map(to:dxa,dya,dt2) map(from:delpc,ptc,wc,divg_d) &
    !$omp map(tofrom:u,vc,v,uc,delp,pt,ua,va,ut,vt,w)
  !$omp parallel do
  do k=1, npz
     call c_sw(sw_corner, se_corner, nw_corner, ne_corner,           &
               rarea, rarea_c, sin_sg, cos_sg, sina_v, cosa_v,       &
               sina_u, cosa_u, fC, rdxc, rdyc, dx, dy, dxc, dyc,     &
               cosa_s, rsin_u, rsin_v, rsin2, dxa, dya,              &
               delpc(isd,jsd,k), delp(isd,jsd,k), ptc(isd,jsd,k),    &
               pt(isd,jsd,k), u(isd,jsd,k), v(isd,jsd,k),            &
               w(isd,jsd,k), uc(isd,jsd,k), vc(isd,jsd,k),           &
               ua(isd,jsd,k), va(isd,jsd,k), wc(isd,jsd,k),          &
               ut(isd,jsd,k), vt(isd,jsd,k), divg_d(isd,jsd,k), dt2)
  enddo
  !$omp end target
```

DPC++ Offload

```fortran
  ! Run the kernel
  call c_sw_dpcpp(isd, ied, jsd, jed, is, ie, js, je, nord, npx, npy,  &
                  npz, do_profile, dt2,                               &
                  sw_corner, se_corner, nw_corner, ne_corner,         &
                  rarea, rarea_c, sin_sg, cos_sg, sina_v, cosa_v,     &
                  sina_u, cosa_u, fC, rdxc, rdyc, dx, dy, dxc, dyc,   &
                  cosa_s, rsin_u, rsin_v, rsin2, dxa, dya,            &
                  delpc, delp, ptc, pt, u, v, w, uc, vc, ua, va, wc,  &
                  ut, vt, divg_d)

  ! !$OMP parallel do schedule(runtime)
  ! do k=1, npz
  !    call c_sw(sw_corner, se_corner, nw_corner, ne_corner,    &
  !              delpc(isd,jsd,k), delp(isd,jsd,k), ptc(isd,jsd,k),   &
  !              pt(isd,jsd,k), u(isd,jsd,k), v(isd,jsd,k),           &
  !              w(isd,jsd,k), uc(isd,jsd,k), vc(isd,jsd,k),          &
  !              ua(isd,jsd,k), va(isd,jsd,k), wc(isd,jsd,k),         &
  !              ut(isd,jsd,k), vt(isd,jsd,k), divg_d(isd,jsd,k), dt2)
  ! enddo
```

Performance Comparison

Testcase	No Offload (+OMP)		Approach 'Outer'			Approach 'Loop'		
	Fortran	C++	OMP	DPC++ GPU	DPC++ CPU	OMP	DPC++ GPU	DPC++ CPU
Default	0.003 s	0.005 s	7.95 s	1.094 s	2.378 s	4.32 s	3.175 s	0.225 s

- Test performed on Intel® DevCloud
- Running on a small test
- Timings exclude memory movement and show pure kernel time
- DPC++ is much slower than Fortran. Why? → 'just in time' compilation

Testing Date: Performance results are **based on testing by Intel as of June 17, 2021** and may not reflect all publicly available security updates.

Configuration Details and Workload Setup: Intel® Xeon® E-2176G Processor with Intel® UHD Graphics P630 on Intel® DevCloud. Ubuntu 20.04.2 LTS, Intel® oneAPI Base Toolkit 2021.2, Intel® oneAPI HPC Toolkit 2021.2. SENA c_sw kernel at https://github.com/NOAA-GSL/SENA-c_sw.

Ahead of time compilation

- Device kernel code is compiled 'just in time' (JIT) at runtime
- A lot of device code → Takes a lot of time
- If hardware is known a priori: Pre-compile (ahead of time, AOT) device code
- Negligible for kernels that are called multiple times, or longer running kernels

CMakeLists.txt

```
cmake_minimum_required( VERSION 3.10 )

project( c_sw LANGUAGES Fortran C CXX)

list( APPEND CMAKE_MODULE_PATH ${CMAKE_CURRENT_SOURCE_DIR}/cmake )
set( CMAKE_DIRECTORY_LABELS ${PROJECT_NAME} )
#set( CMAKE_EXE_LINKER_FLAGS "-g -lifcore" )
set( CMAKE_EXE_LINKER_FLAGS "-g -lifcore -fsycl-targets=spir64_x86_64-unknown-unknown-sycldevice \
   -Xs \"-march=sse4.2\"" )
#set( CMAKE_EXE_LINKER_FLAGS "-g -lifcore -fsycl-targets=spir64_gen-unknown-unknown-sycldevice \
#    -Xs \"-device gen9\"" )


enable_testing()

include(${PROJECT_NAME}_compiler_flags)

find_package( OpenMP COMPONENTS C Fortran )
find_package( NetCDF REQUIRED COMPONENTS C Fortran )

add_subdirectory(src)
add_subdirectory(test)

set_target_properties( ${PROJECT_NAME} PROPERTIES LINKER_LANGUAGE CXX )
```

```
add_executable( ${PROJECT_NAME} ${OBJS} ${c_sw_src_files} )

#target_compile_options(${PROJECT_NAME} PUBLIC $<$<COMPILE_LANGUAGE:CXX>:-v
#  -fsycl-targets=spir64_gen-unknown-unknown-sycldevice>)
target_compile_options(${PROJECT_NAME} PUBLIC $<$<COMPILE_LANGUAGE:CXX>:-v
    -fsycl-targets=spir64_x86_64-unknown-unknown-sycldevice>)
```

src/CMakeLists.txt

Performance Comparison

Testcase	No Offload (+OMP)		Approach 'Outer'			Approach 'Loop'		
	Fortran	C++	OMP*	DPC++ GPU	DPC++ CPU	OMP*	DPC++ GPU	DPC++ CPU
Default	0.003 s	0.005 s	7.95 s	1.094 s	2.378 s	4.32 s	3.175 s	0.225 s
AOT	0.003 s	0.005 s	7.95 s	0.094 s	0.042 s	4.32 s	3.049 s	0.079 s

- Gains from AOT more prominent if there is more device code
- DPC++ outperforms OMP
- Offload still slower due to low GPU usage and the device used
- *Known issue with AOT, OMP offload and Gen9 graphics

Testing Date: Performance results are **based on testing by Intel as of June 17, 2021** and may not reflect all publicly available security updates.

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Performance Comparison

Testcase	No Offload (+OMP)		Approach 'Outer'			Approach 'Loop'		
	Fortran	C++	OMP	DPC++ GPU	DPC++ CPU	OMP	DPC++ GPU	DPC++ CPU
Default	0.003 s	0.005 s	7.95 s	1.094 s	2.378 s	4.32 s	3.175 s	0.225 s
AOT	0.003 s	0.005 s	7.95 s	0.094 s	0.042 s	4.32 s	3.049 s	0.079 s
Large Case	4.239 s	3.95 s	11.66 s	16.33 s	3.94 s	60 s	7.73 s	9.29 s

- 'Large Case' test is ~330 times the size of 'Default' test
- AOT is also used in these tests (except OMP)

Testing Date: Performance results are **based on testing by Intel as of June 17, 2021** and may not reflect all publicly available security updates.

Configuration Details and Workload Setup: Intel® Xeon® E-2176G Processor with Intel® UHD Graphics P630 on Intel® DevCloud. Ubuntu 20.04.2 LTS, Intel® oneAPI Base Toolkit 2021.2, Intel® oneAPI HPC Toolkit 2021.2. SENA c_sw kernel at https://github.com/NOAA-GSL/SENA-c_sw.

Summary

- Fortran – DPC++ migration possible and feasible
- Still requires Fortran – C++ migration for kernel code
- Leveraging C++ in kernel code and implicit data movement between host and device allows neat code and easy migration
- Performance in such a first approach might not be ideal
- One of the core strengths of DPC++ is C++

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Resources

- NOAA c_sw kernel - https://github.com/NOAA-GSL/SENA-c_sw
- Intel® oneAPI – https://software.intel.com/oneapi
- Intel® DevCloud for oneAPI – https://devcloud.intel.com/oneapi

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