Porting the parallel Nek5000 application to GPU accelerators with OpenMP4.5

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EPiGRAM

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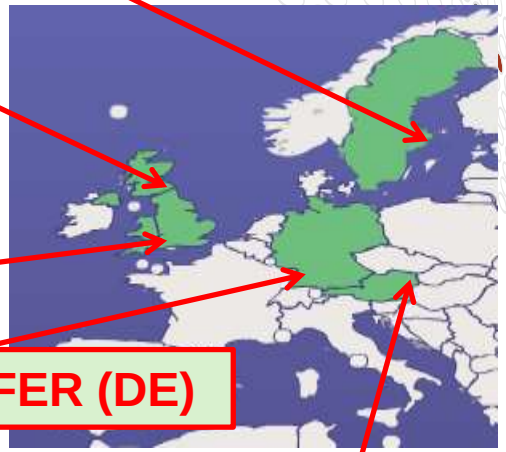

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Contents of the talk

- A brief introduction to accelerator directives
- Porting the NekBone mini-app to OpenMP
- Porting the Nek5000 code from OpenACC to OpenMP

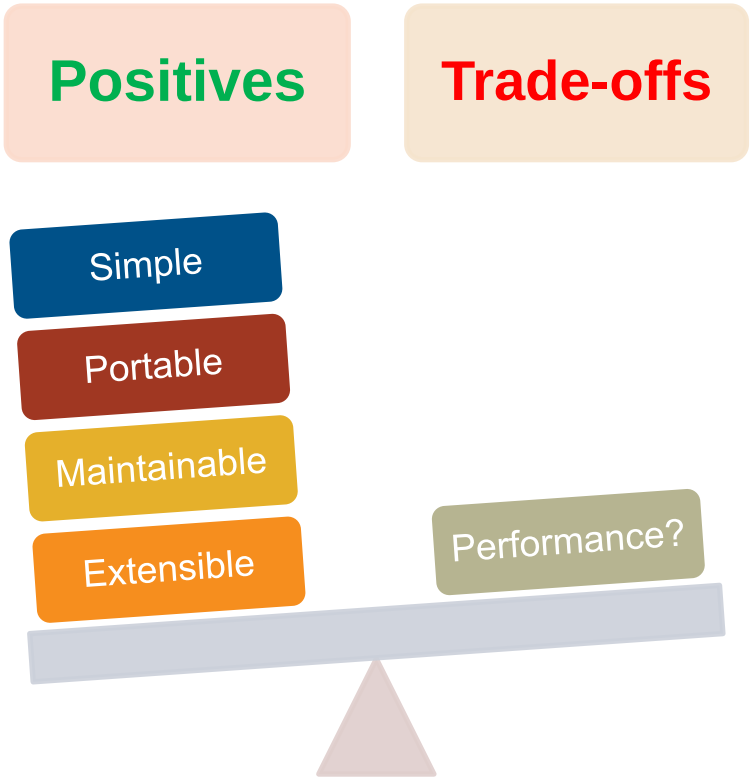
Directive based programming

Add directives to code

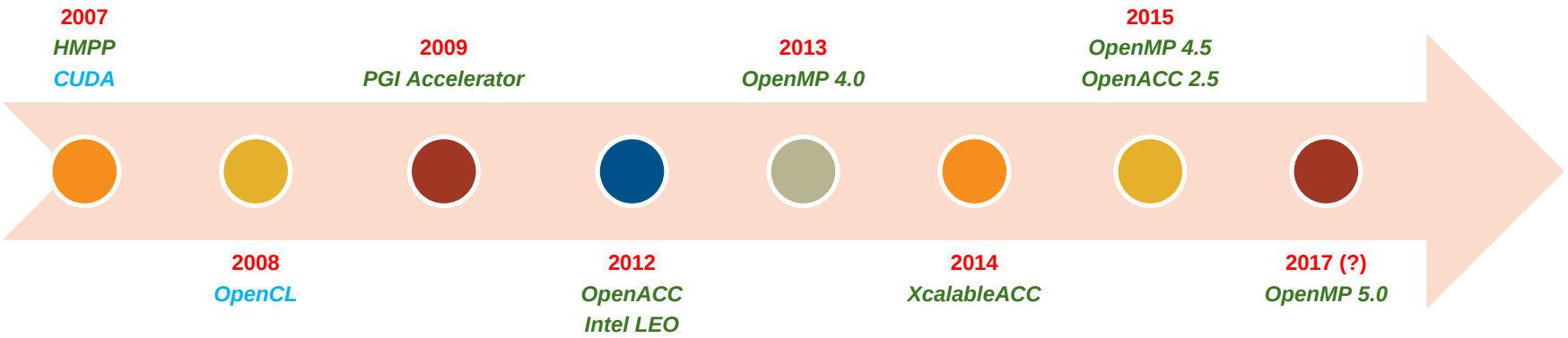
Compile for CPU as usual

Or compile for accelerator

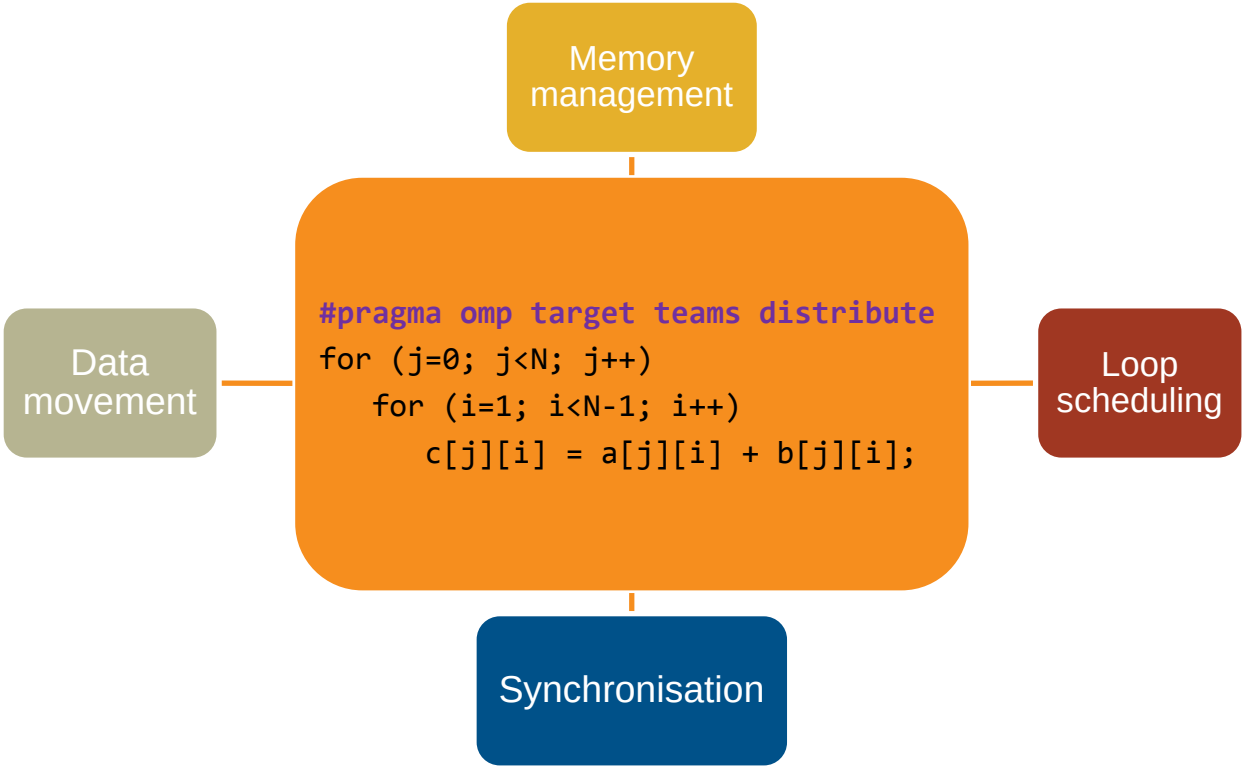
Why use accelerator directive models?



Accelerator directives are not new



A simple example



target teams distribute

- **target creates an offload kernel**
- **teams creates a "league" of "threadteams"**
  - Similar to a parallel region, but can't synchronise
  - Compiler chooses number of teams and threads per team
  - Can over-ride this with optional clauses
- **distribute partitions loop iterations over threads**
  - Multiple loops can be partitioned (unlike host OpenMP)

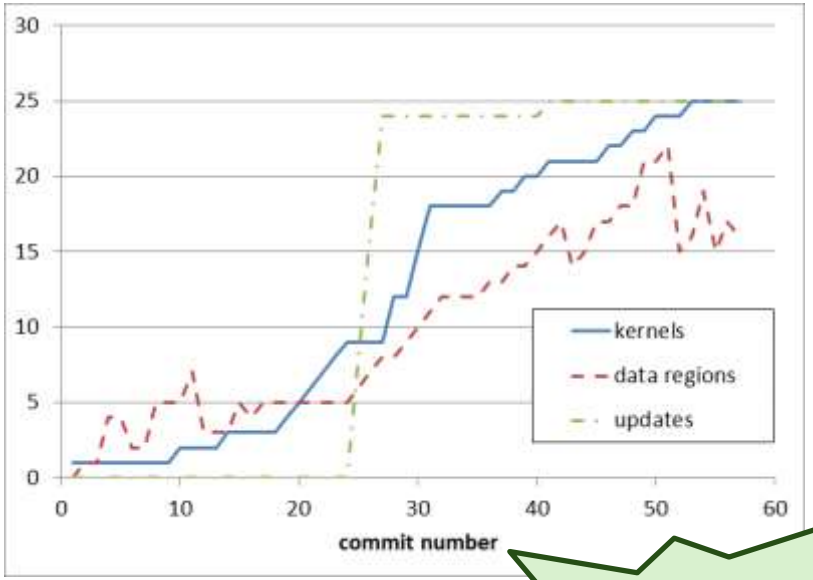
NekBone and Nek5000

Nek5000 and NekBone

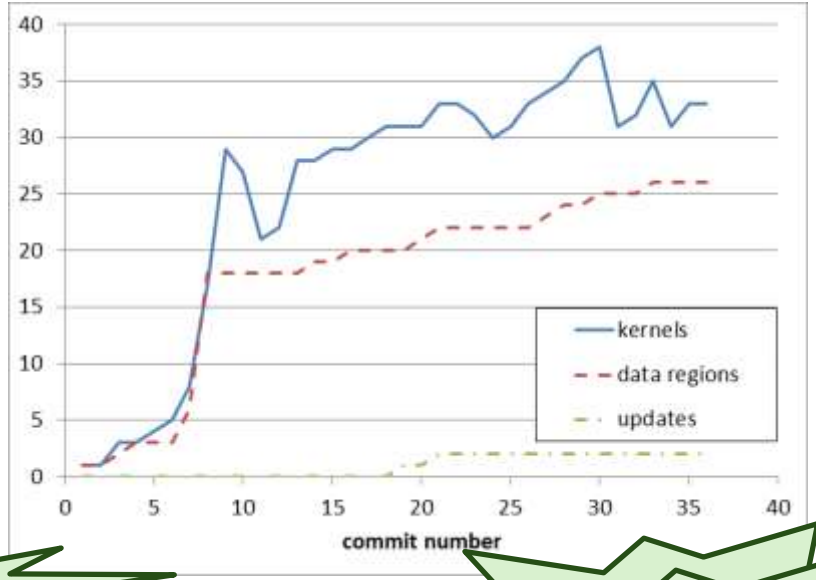
- **Nek5000: CFD code**
  - simulates incompressible fluids.
  - solves Navier-Stokes equations
  - semi-spectral element method.
- **~70k lines of code:**
  - 90% in Fortran 77
  - 10% in C (comms).
  - Parallelised with MPI
- **NekBone mini-app**
  - captures this in 11k lines

How many directives?

OpenMP



OpenACC



420 Mflops

G2G MPI

NekBone kernel performance (OpenMP4.0)

local_oz

```
G----------< !$omp target teams distribute
G            !$omp&  private(e_back,e_front)
G g---------< do e_z =1,mz-1
G g C-------<  do e_y = 1,my
G g C C-----<   do e_x = 1,mx
```

```
G----------< !$omp target teams distribute collapse(3)
G            !$omp&  private(e_back,e_front)
G C---------< do e_z =1,mz-1
G C C-------<  do e_y = 1,my
G C C g-----<   do e_x = 1,mx
G C C g          e_back = e_x + mx*(e_y-1)+mx*my*(e_z-1)
G C C g          e_front = e_back+mx*my
G C C g r2--<    do i=1,n_shared
G C C g r2        w(l_face_z_back(i),e_back)= &
G C C g r2           w(l_face_z_back(i),e_back)+ &
G C C g r2           w(l_face_z_front(i),e_front)
G C C g r2        w(l_face_z_front(i),e_front) = &
G C C g r2           w(l_face_z_back(i),e_back)
G C C g r2-->    enddo
G C C g----->   enddo
G C C------->  enddo
G C--------->enddo
G----------->
```

863µs→142µs

```
G----------< !$acc parallel loop

G g---------< do e_z =1,mz-1
G g 3-------<  do e_y = 1,my
G g 3 4-----<   do e_x = 1,mx
```

```
G----------< !$acc parallel loop collapse(3)

G C---------< do e_z =1,mz-1
G C C-------<  do e_y = 1,my
G C C g-----<   do e_x = 1,mx
G C C g          e_back = e_x + mx*(e_y-1)+mx*my*(e_z-1)
G C C g          e_front = e_back+mx*my
G C C g r2-<     do i=1,n_shared
G C C g r2        w(l_face_z_back(i),e_back)= &
G C C g r2           w(l_face_z_back(i),e_back)+ &
G C C g r2           w(l_face_z_front(i),e_front)
G C C g r2        w(l_face_z_front(i),e_front) = &
G C C g r2           w(l_face_z_back(i),e_back)
G C C g r2->     enddo
G C C g----->   enddo
G C C------->  enddo
G C--------->enddo
G----------->
```

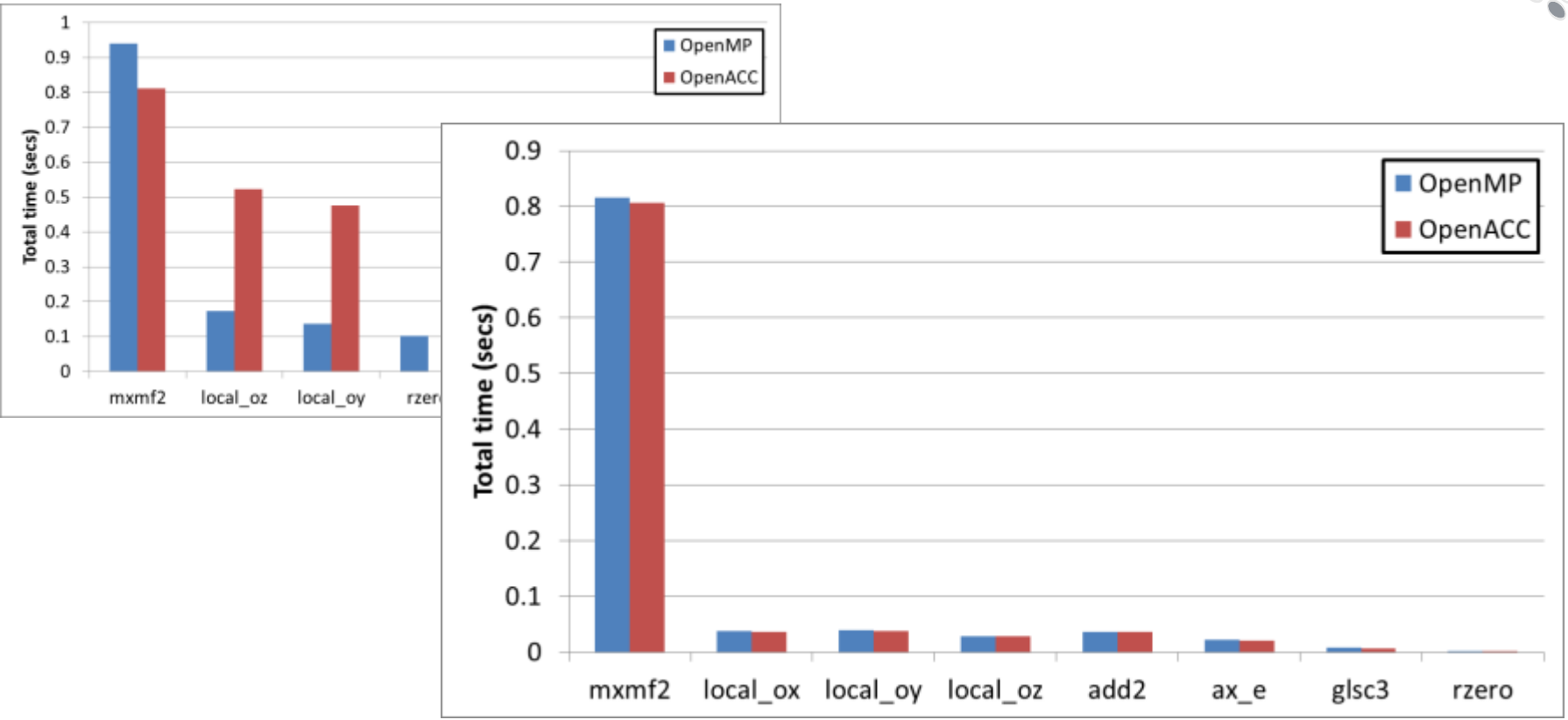
2592µs→141µs

mxmf2

```
G---------< !$omp target teams distribute
G g-------< DO j = 1,n3
G g g-----<  DO i = 1,n1
G g g         c(i,j) = 0
G g g r4--<   DO k = 1,n2
G g g r4       c(i,j) = c(i,j) + a(i,k)*b(k,j)
G g g r4-->   ENDDO
G g g----->  ENDDO
G g------> ENDDO
G---------> !$omp end target teams d
```

```
G---------< !$acc parallel loop
G g-------< DO j = 1,n3
G g g-----<  DO i = 1,n1
G g g         c(i,j) = 0
G g g r4--<   DO k = 1,n2
G g g r4       c(i,j) = c(i,j) + a(i,k)*b(k,j)
G g g r4-->   ENDDO
G g g----->  ENDDO
G g------> ENDDO
G---------> !$acc end parallel loop
```

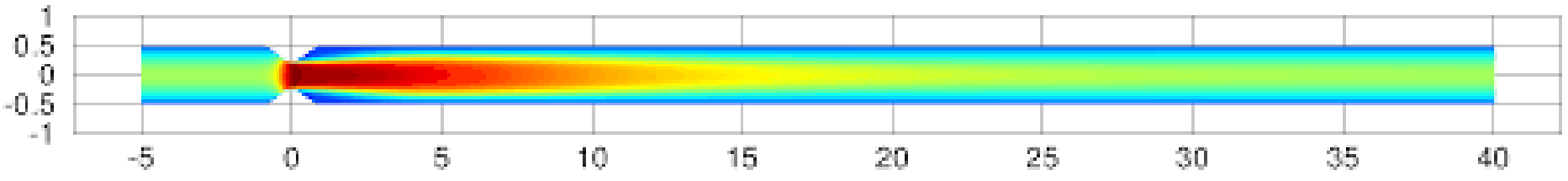
NekBone performance after tuning



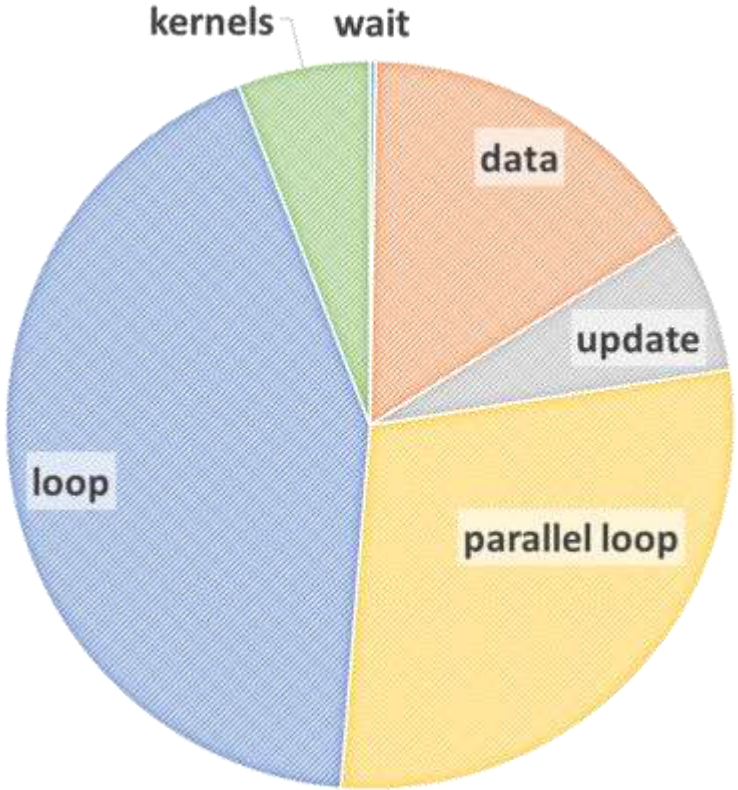
Nek5000

Nek5000

- **Already ported to OpenACC**
- **Migrating to OpenMP?**
  - Can we do this without losing performance?
  - What are the challenges in migrating?
  - What are the advantages of migration



OpenACC directive audit



- **74000 source lines**
  - 60000 lines of code
- **691 directive lines:**
  - 390 directives
  - 101 continuation lines
  - 200 end directives
- **155 loc/directive**
- **Traffic lights and alarm bells:**
  - data, update, parallel loop, wait
  - loop
  - kernels

Planning the migration with the calltree

- 13 source files
- Interoperability is key

```
Table 1:  Calltree View with Callsite Line Numbers

  Time% |      Time |     Calls |Calltree
        |           |           | PE=HIDE

 100.0% | 25.213824 |        -- |Total
|  54.8% | 13.811506 |         -- |nekton_:drive.f:line.50
||  54.8% | 13.811480 |          -- |nek_solve_:drive1.f:line.260
3||  40.3% | 10.164313 |           -- |nek_solve_.ACC_DATA_REGION@li.260:drive1.f:line.328
4|||  39.5% |  9.966259 |            -- |nek__multi_advance_:drive1.f:line.446
5|||       |           |               | nek_advance_:drive1.f:line.384
6|||       |           |               |  fluid_:drive2.f:line.758
7||||||  31.2% |  7.869682 |           -- |plan4_acc_:plan4.f:line.532
8|||||||  28.5% |  7.174353 |            -- |plan4_acc_.ACC_DATA_REGION@li.532:plan4.f:line.453
9|||||||  28.5% |  7.174286 |             -- |hsolve_acc_:navier4.f:line.952
10|||||||  28.5% |  7.174220 |             -- |hmholtz_acc_:hmholtz.f:line.1521
11|||||||||  28.4% |  7.163318 |             -- |hmholtz_acc_.ACC_DATA_REGION@li.1521:hmholtz.f:line.1468
12|||||||||  28.4% |  7.163282 |             -- |cggo_acc_:hmholtz.f:line.1581
13||||||||||   7.9% |  1.991531 |              -- |cggo_acc_.ACC_DATA_REGION@li.1581:hmholtz.f:line.1668
14||||||||||   7.9% |  1.981263 |              -- |fdm_h1_acc_:hmholtz.f:line.2161
15|||||||||||   5.0% |  1.249621 |               -- |fdm_h1_acc_.ACC_DATA_REGION@li.2161:hmholtz.f:line.2352
16|||||||||||   2.6% |  0.650272 |               -- |dssum_acc_:dssum.f:line.1002
17||||||||||||   2.1% |  0.519627 |   5,349.0 |dssum_acc_.ACC_DATA_REGION@li.1002:dssum.f:line.1002
18||||||||||||   0.0% |  0.007974 |   5,349.0 |dssum_acc_.ACC_COPY@li.1002:dssum.f:line.1002
```

Basic example

- **Both directives**
- **private scalars**
- **thread_limit**

- **a7_dudxyz.f**

```
                #ifdef _ACCEL_OPENMP
G-----------< !$omp target teams distribute collapse(4)
G             !$omp& private(tmpx) thread_limit(VLENGTH)
G             #endif
G             #ifdef _ACCEL_OPENACC
D             !$acc parallel loop collapse(4)
D             !$acc& private(tmpx) vector_length(VLENGTH)
G             #endif
G C---------< DO E = 1,NEL
G C C-------<  DO K = 1,NZ1
G C C C-----<   DO J = 1,NY1
G C C C g---<    DO I = 1,NX1
G C C C g         TMPX = 0.0
G C C C g 6-<     DO L = 1,NX1
G C C C g 6        TMPX = TMPX + DXTM1(L,I)*U(L,J,K,E)
G C C C g 6->     ENDDO
G C C C g         DU(I,J,K,E) = TMPX*RM1(I,J,K,E)
G C C C g--->    ENDDO
G C C C----->   ENDDO
G C C------->  ENDDO
G C--------> ENDDO
```

Providing loop information

- collapse

```
G------------< !$omp target teams distribute
G g----------< DO IE=1,NEL
G g            !$omp simd collapse(3)
D              !$acc loop collapse(3)
G g C--------<  IZ=1,NZ1
G g C C------<  DO IY=1,NY1
G g C C g----<   DO IX=1,NX1
G g C C g         DPCM1(IX,IY,IZ,IE) = 0.0
G g C C g r4-<    DO IQ=1,NX1
G g C C g r4       DPCM1(IX,IY,IZ,IE) += ...
G g C C g r4->    ENDDO
G g C C g---->   ENDDO
G g C C------>  ENDDO
G g C-------->ENDDO
```

- a2_setprec.f

Providing loop information (2)

- Reductions on inner loops
- forced collapse

```
G-----------< !$omp target teams distribute private(h1b)
G g---------< DO ie=1,nel
G g           h1b = 0
G g          !$omp simd collapse(3) reduction(+:h1b)
D            !$acc loop reduction(+:h1b)
G g g-------<  DO i3=1,nz1
G g g C-----<   DO i2=1,ny1
G g g C Cr4-<    DO i1=1,nx1
G g g C Cr4       h1b = h1b + h1(i1,i2,i3,ie)
G g g C Cr4->    ENDDO
G g g C----->   ENDDO
G g g------->  ENDDO
```

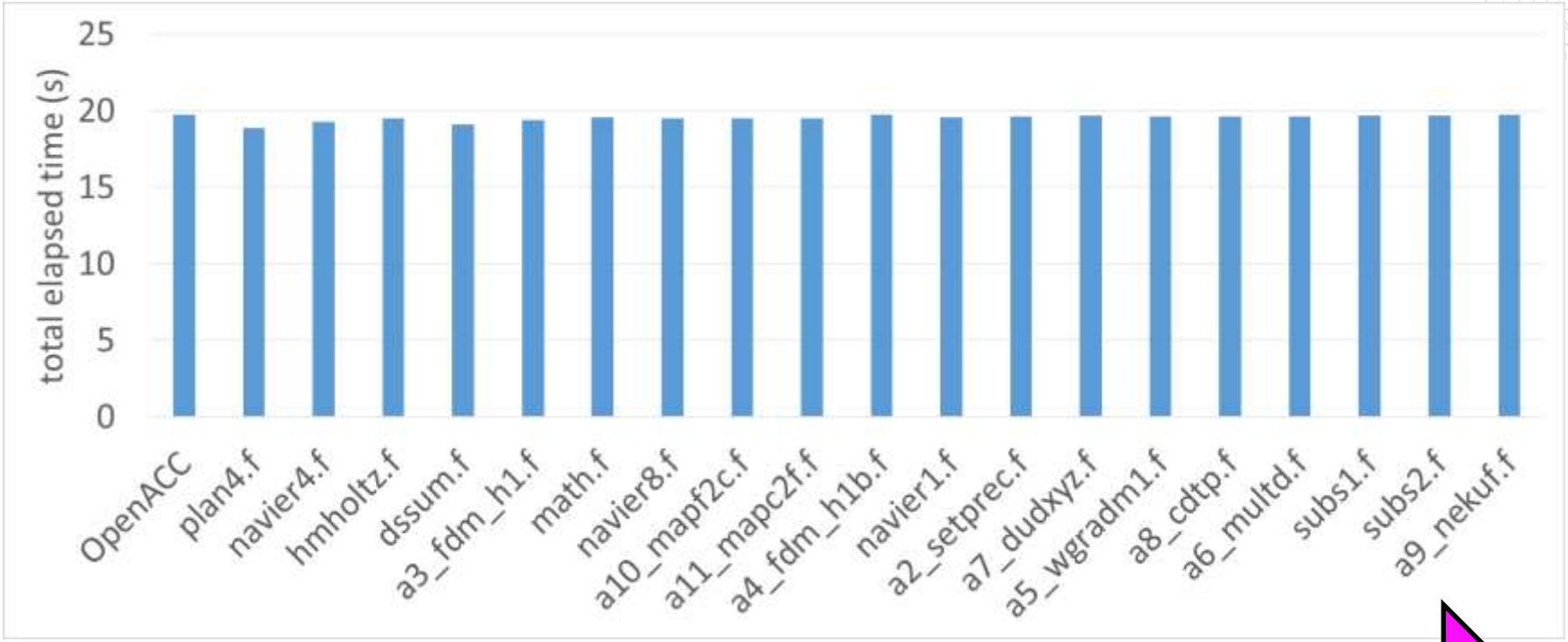
- a4_fdm_h1b.f

Providing loop information (3)

- **No equivalent:**
  - Elimination process
  - Compiler directives
    - CCE: !dir$ novector
- **a10_mapf2c.f**

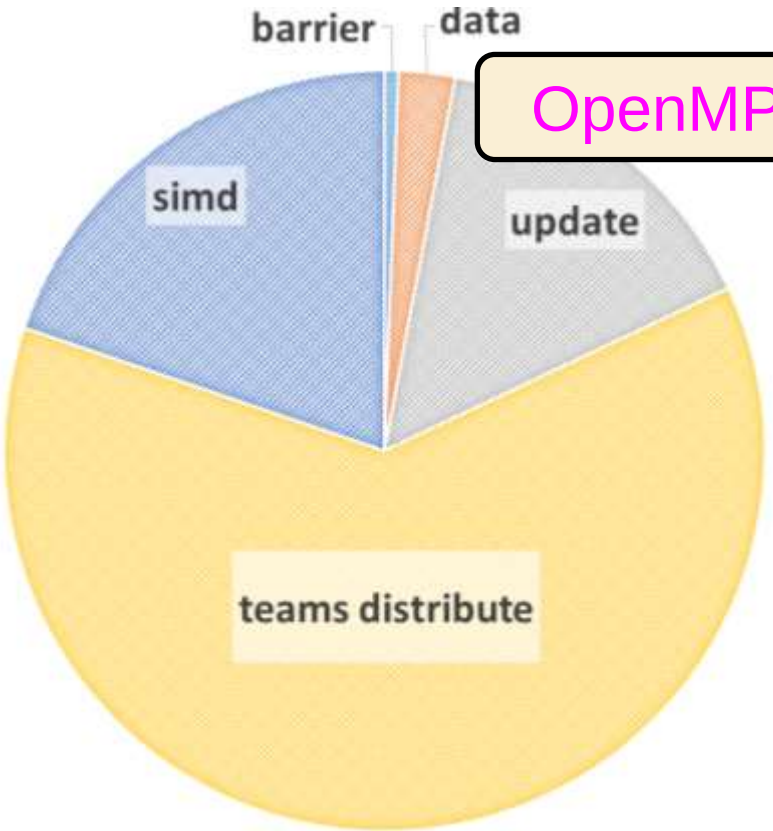
```
G------------< !$omp target teams distribute
G------------< !$omp& simd collapse(4)
G C----------< DO e = 1,nelv
G C C--------<  DO k = 1,nz1
G C C C------<   DO j = 1,ny1
G C C C g----<    DO i = 1,n2
G C C C g          tmpv = 0.0
D                !$acc loop seq
G C C C g r4-<     DO l = 1,nx1
G C C C g r4        tmpv = tmpv + ...
G C C C g r4->     ENDDO
G C C C g          v2(i,j,k,e) = tmpv
G C C C g---->    ENDDO
G C C C------>   ENDDO
G C C-------->  ENDDO
G C---------->  ENDDO
```

Nek5000 performance during migration



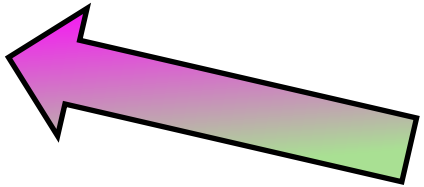
Porting time

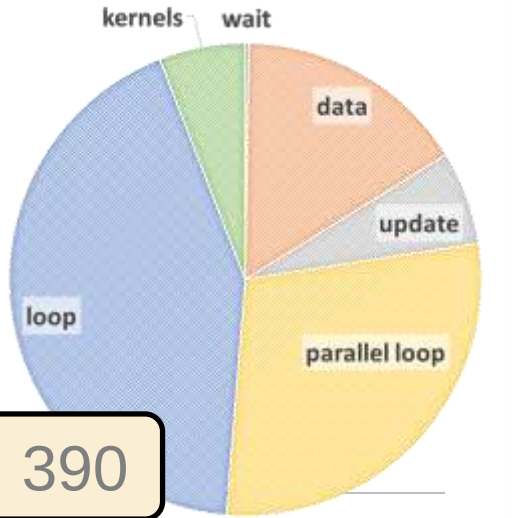
OpenMP directive audit



OpenMP: 167

- **Fewer:**
  - data regions
  - loop directives

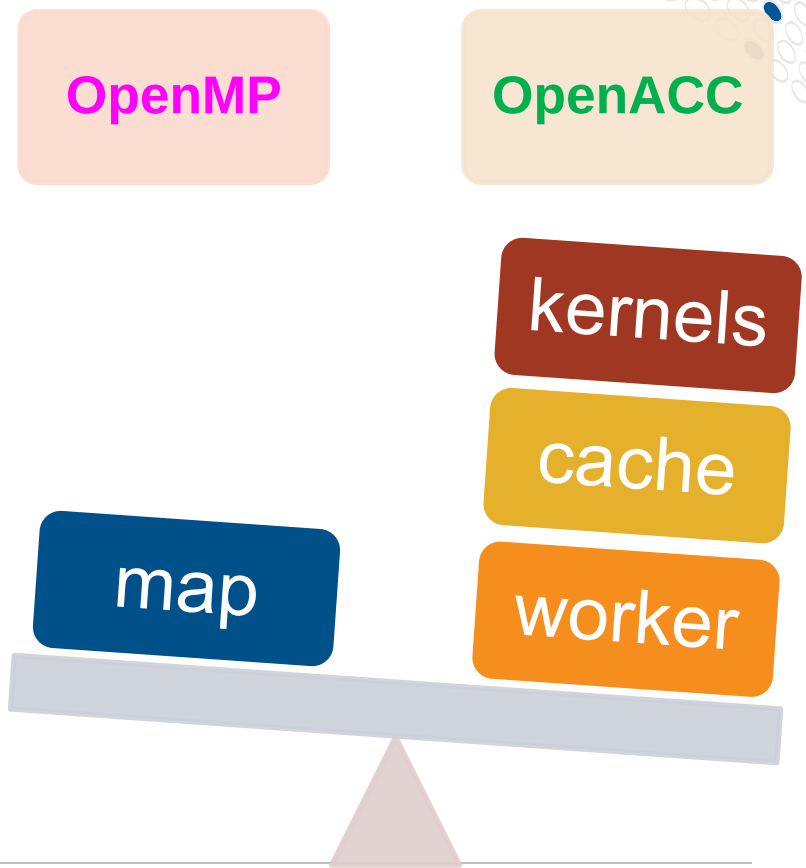




OpenACC: 390

OpenMP4.5 versus OpenACC

- **OpenMP4.5 a close match**
  - added:
    - use_device_ptr
    - scalars firstprivate by default
    - unstructured data regions
    - better async control



OpenMP4.5 versus OpenACC

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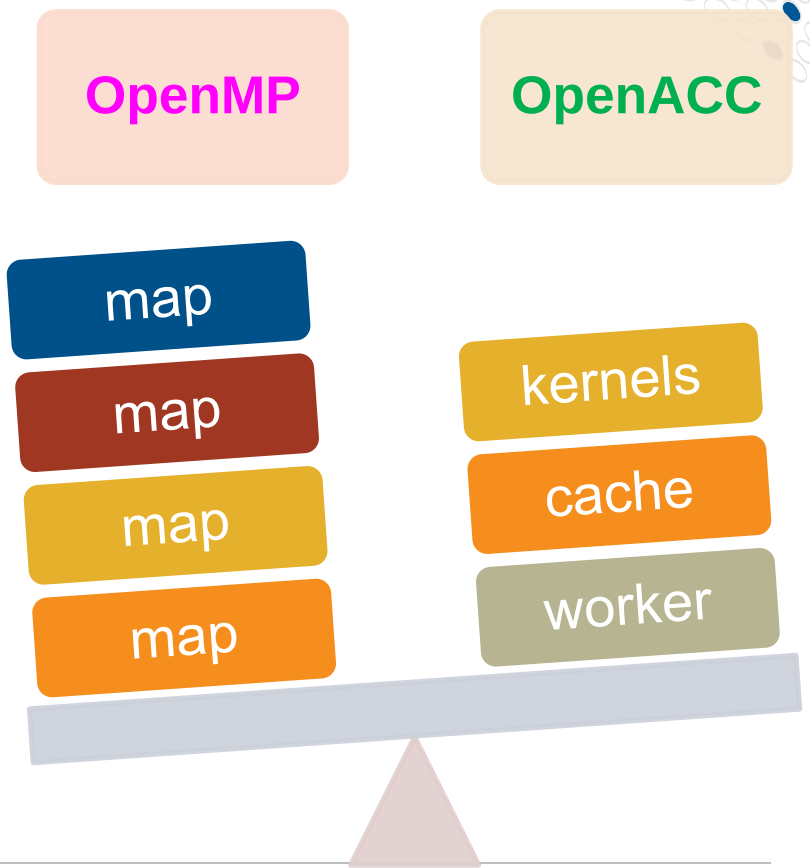

Conclusions

- **Directives offer productive performance-portability**
  - Nek5000/NekBone: 1 directive per 160 lines of code
- **OpenMP device constructs: mature programming model**
- **OpenMP device constructs can (should) be performant**
  - CCE: default comparable and often better than OpenACC
  - Fewer tuning clauses, but does not appear to be a problem
- **Straightforward migration path: OpenACC ⇔ OpenMP**
  - Interoperability is a great help for incremental porting
  - Subtleties but nothing deal-breaking
  - OpenMP tends to use fewer directives, more maintainable

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