First experiences porting a parallel application to a hybrid supercomputer with OpenMP 4.0 device constructs

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EPiGRAM

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Contents of the talk

- A brief introduction to accelerator directives
- Porting a simple example
- Porting the NekBone code

Directive based programming

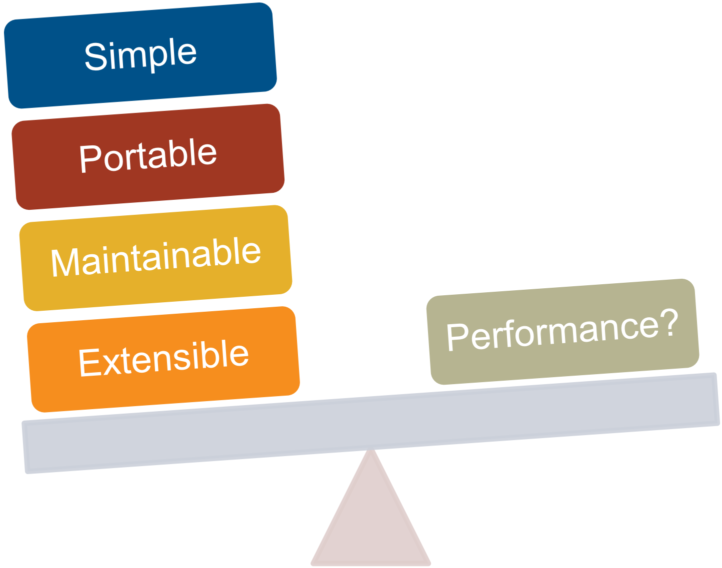
Add directives to code

Compile for CPU as usual

Or compile for accelerator

Why use accelerator directive models?

Positives | **Trade-offs**



Accelerator directives are not new

2007
HMPP
CUDA

2008
OpenCL

2009
PGI Accelerator

2012
OpenACC
Intel LEO

2013
OpenMP 4.0

2014
XcalableACC

2015 (?)
OpenMP 4.1
OpenACC 2.5

A simple example

Memory management

Data movement

```
#pragma omp target teams \
            distribute
for (j=0; j<N; j++)
 for (i=1; i<N-1; i++)
  c[j][i]=a[j][i]+b[j][i];
```

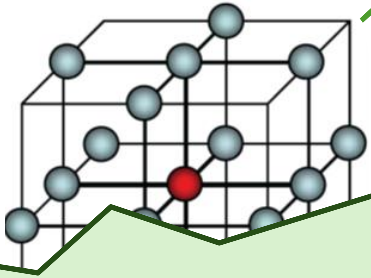
Loop scheduling

Synchronisation

target teams distribute

- **target creates an offload kernel**
- **teams creates a "league" of "threadteams"**
  - 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)
- **CCE v8.4 targets Nvidia GPUs**
  - distribute fully partitions iterations over all levels of parallelism
  - "distribute parallel simd" not needed
    - distribute simd can be used for tuning

The Himeno code



- Poisson solver
  - 3d
  - iterative loop
- Memory intensive
  - 19pt stencil
  - b/w bound
- Small
  - 250 lines
  - Fortran, C

1thread: 3.3 Gflops
10 threads: 11.1 Gflops

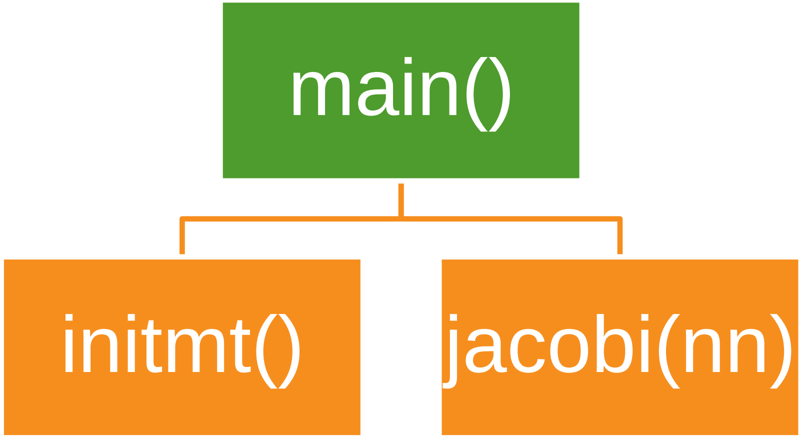
Acceleration planning

- **Understand call tree**
- **Inspection or profiling**
  - e.g. CrayPAT

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

  Time% |     Time | Calls |Calltree

 100.0% | 4.432070 |    -- |Total
|-------------------------------------------------------------
|  91.9% | 4.070905 |    -- |main_:himeno_F_v0.F90:line.171
|  91.9% | 4.070905 |   1.0 | jacobi_:himeno_F_v0.F90:line.241
|   4.9% | 0.215086 |    -- |main_:himeno_F_v0.F90:line.118
|   4.9% | 0.215086 |   1.0 | initmt_:himeno_F_v0.F90:line.189
|   3.1% | 0.136999 |    -- |main_:himeno_F_v0.F90:line.150
|   3.1% | 0.136999 |   1.0 | jacobi_:himeno_F_v0.F90:line.241
|=============================================================
```



Understanding the loops

- Loopnest dominated?
- Iteration counts
- Granularity

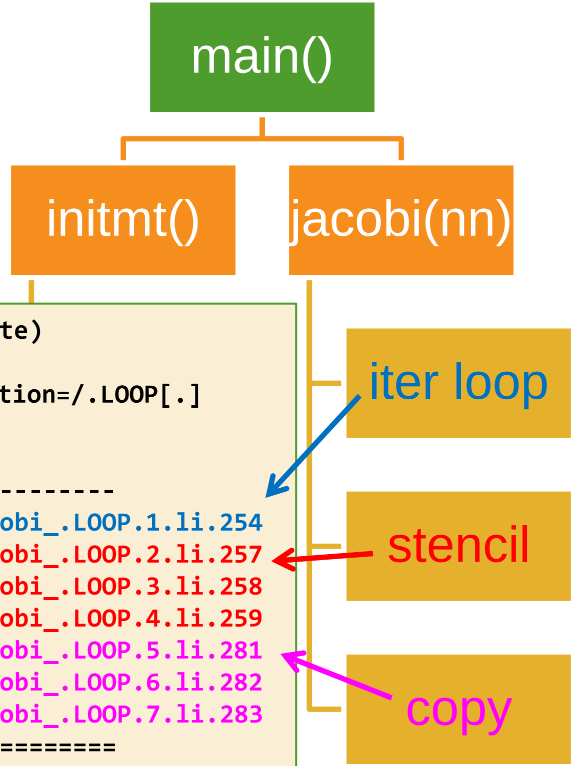


Table 2: Inclusive and Exclusive Time in Loops (from -hprofile_generate)

Loop Incl Time%	Loop Incl Time	Time (Loop Adj.)	Loop Hit	Loop Trips Avg	Loop Trips Min	Loop Trips Max	Function=/.LOOP[.]
95.3%	3.957659	0.000022	2	51.5	3	100	jacobi_.LOOP.1.li.254
81.8%	3.397517	0.000653	103	126.0	126	126	jacobi_.LOOP.2.li.257
81.8%	3.396864	0.031151	12,978	126.0	126	126	jacobi_.LOOP.3.li.258
81.1%	3.365713	3.365713	1,635,228	254.0	254	254	jacobi_.LOOP.4.li.259
13.5%	0.560120	0.000175	103	126.0	126	126	jacobi_.LOOP.5.li.281
13.5%	0.559945	0.080416	12,978	126.0	126	126	jacobi_.LOOP.6.li.282
11.5%	0.479529	0.479529	1,635,228	254.0	254	254	jacobi_.LOOP.7.li.283

Accelerating the stencil loopnest

```
DO k = 2,kmax-1
 DO j = 2,jmax-1
  DO i = 2,imax-1
   s0 = a(i,j,k,1) *   p(i+1,j  ,k  ) &
      + a(i,j,k,2) *   p(i  ,j+1,k  ) &
      + a(i,j,k,3) *   p(i  ,  j,k+1) &
      + b(i,j,k,1) * ( p(i+1,j+1,k  ) - p(i+1,j-1,k  ) &
                     - p(i-1,j+1,k  ) + p(i-1,j-1,k  ) ) &
      + b(i,j,k,2) * ( p(i  ,j+1,k+1) - p(i  ,j-1,k+1) &
                     - p(i  ,j+1,k-1) + p(i  ,j-1,k-1)) &
      + b(i,j,k,3) * ( p(i+1,j  ,k+1) - p(i-1,j  ,k+1) &
                     - p(i+1,j  ,k-1) + p(i-1,j  ,k-1)) &
      + c(i,j,k,1) *   p(i-1,j  ,k  ) &
      + c(i,j,k,2) *   p(i  ,j-1,k  ) &
      + c(i,j,k,3) *   p(i  ,j  ,k-1) &
      + wrk1(i,j,k)

   ss = ( s0 * a(i,j,k,4) - p(i,j,k) ) * bnd(i,j,k)
   gosa = gosa + ss*ss
   wrk2(i,j,k) = p(i,j,k) + omega * ss
  ENDDO
 ENDDO
ENDDO
```

Accelerating the stencil loopnest

```
!$omp target teams distribute reduction(+:gosa) private(s0,ss)
DO k = 2,kmax-1
 DO j = 2,jmax-1
  DO i = 2,imax-1
   S0 = a(i,j,k,1) *   p(i+1,j  ,k  ) &
      + a(i,j,k,2) *   p(i  ,j+1,k  ) &
      + a(i,j,k,3) *   p(i  ,  j,k+1) &
      + b(i,j,k,1) * ( p(i+1,j+1,k  ) - p(i+1,j-1,k  ) &
                     - p(i-1,j+1,k  ) + p(i-1,j-1,k  ) ) &
      + b(i,j,k,2) * ( p(i  ,j+1,k+1) - p(i  ,j-1,k+1) &
                     - p(i  ,j+1,k-1) + p(i  ,j-1,k-1)) &
      + b(i,j,k,3) * ( p(i+1,j  ,k+1) - p(i-1,j  ,k+1) &
                     - p(i+1,j  ,k-1) + p(i-1,j  ,k-1)) &
      + c(i,j,k,1) *   p(i-1,j  ,k  ) &
      + c(i,j,k,2) *   p(i  ,j-1,k  ) &
      + c(i,j,k,3) *   p(i  ,j  ,k-1) &
      + wrk1(i,j,k)

   ss = ( s0 * a(i,j,k,4) - p(i,j,k) ) * bnd(i,j,k)
   gosa = gosa + ss*ss
   wrk2(i,j,k) = p(i,j,k) + omega * ss
  ENDDO
 ENDDO
ENDDO
!$omp end target teams distribute
```

Accelerating the stencil loopnest

```
+ 1 G----------< !$omp target teams distribute reduction(+:gosa) private(s0,ss)
  1 G g--------< DO k = 2,kmax-1
+ 1 G g b------<  DO j = 2,jmax-1
  1 G g b gb---<   DO i = 2,imax-1
  1 G g b gb        S0 = a(i,j,k,1) *   p(i+1,j  ,k  ) &
  1 G g b gb           + a(i,j,k,2) *   p(i  ,j+1,k  ) &
  1 G g b gb           + a(i,j,k,3) *   p(i  ,  j,k+1) &
  1 G g b gb           + b(i,j,k,1) * ( p(i+1,j+1,k  ) - p(i+1,j-1,k  ) &
  1 G g b gb                          - p(i-1,j+1,k  ) + p(i-1,j-1,k  ) ) &
  1 G g b gb           + b(i,j,k,2) * ( p(i  ,j+1,k+1) - p(i  ,j-1,k+1) &
  1 G g b gb                          - p(i  ,j+1,k-1) + p(i  ,j-1,k-1)) &
  1 G g b gb           + b(i,j,k,3) * ( p(i+1,j  ,k+1) - p(i-1,j  ,k+1) &
  1 G g b gb                          - p(i+1,j  ,k-1) + p(i-1,j  ,k-1)) &
  1 G g b gb           + c(i,j,k,1) *   p(i-1,j  ,k  ) &
  1 G g b gb           + c(i,j,k,2) *   p(i  ,j-1,k  ) &
  1 G g b gb           + c(i,j,k,3) *   p(i  ,j  ,k-1) &
  1 G g b gb           + wrk1(i,j,k)
  1 G g b gb
  1 G g b gb        ss = ( s0 * a(i,j,k,4) - p(i,j,k) ) * bnd(i,j,k)
  1 G g b gb        gosa = gosa + ss*ss
  1 G g b gb        wrk2(i,j,k) = p(i,j,k) + omega * ss
  1 G g b gb--->   ENDDO
  1 G g b------>  ENDDO
  1 G g--------> ENDDO
  1 G----------> !$omp end target teams distribute
```

Accelerating the stencil loopnest

```
272.  + 1 G----------< !$omp target teams distribute reduction(+:gosa) private(s0,ss)  map(from:wrk2)
273.    1 G g--------< DO k = 2,kmax-1
274.  + 1 G g b------<  DO j = 2,jmax-1
275.    1 G g b gb---<   DO i = 2,imax-1
276.    1 G g b gb         S0 = a(i,j,k,1) *   p(i+
277.    1 G g b gb            + a(i,j,k,2) *   p(i
278.    1 G g b gb            + a(i,j,k,3) *   p(i
279.    1 G g b gb            + b(i,j,k,1) * ( p(i+
280.    1 G g b gb                           - p(i-
281.    1 G g b gb            + b(i,j,k,2) * ( p(i
282.    1 G g b gb                           - p(i
283.    1 G g b gb            + b(i,j,k,3) * ( p(i+
284.    1 G g b gb                           - p(i+
285.    1 G g b gb            + c(i,j,k,1) *   p(i-
286.    1 G g b gb            + c(i,j,k,2) *   p(i
287.    1 G g b gb            + c(i,j,k,3) *   p(i
288.    1 G g b gb            + wrk1(i,j,k)
289.    1 G g b gb
290.    1 G g b gb         ss = ( s0 * a(i,j,k,4) -
291.    1 G g b gb         gosa = gosa + ss*ss
292.    1 G g b gb         wrk2(i,j,k) = p(i,j,k) +
293.    1 G g b gb--->   ENDDO
294.    1 G g b------>  ENDDO
295.    1 G g-------->  ENDDO
296.    1 G----------> !$omp end target teams dist
```

```
ftn-6405 ftn: ACCEL File = himeno_F_v1.F90, Line = 272
  A region starting at line 272 and ending at line 296 was placed on
the accelerator.

ftn-6418 ftn: ACCEL File = himeno_F_v1.F90, Line = 272
  If not already present: allocate memory and copy whole array "p"
to accelerator, free at line 296 (acc_copyin).

Similar messages for a,b,c,bnd,wrk1.

ftn-6420 ftn: ACCEL File = himeno_F_v1.F90, Line = 272
  If not already present: allocate memory and copy wh    array
"wrk2" to accelerator, copy back a   line 29

ftn-6430 ftn: ACCEL File = him
  A loop starting at line 27                           ead
blocks.

ftn-6049 ftn: SCALAR File = himeno_  v1.F90, Line = 274
  A loop starting at line 274 was blocked with block size 8.

ftn-6430 ftn: ACCEL File = himeno_F_v1.F90, Line = 275
  A loop starting at line 275 was partitioned across the 128 threads
within a threadblock.
```

~~3.3 Gflops~~

1.5 Gflops

Runtime feedback: CRAY_ACC_DEBUG

```
ACC: Start transfer 14 items from himeno_F_v1.F90:158
ACC:       allocate, copy to acc 'p' (34213896 bytes)
ACC:       allocate 'wrk2' (34213896 bytes)
ACC:       allocate, copy to acc 'imax' (4 bytes)

ACC:       allocate reusable <internal> (8 bytes)
ACC:       allocate reusable, copy to acc <internal> (4 bytes)
ACC:       allocate reusable <internal> (1008 bytes)
ACC: End transfer (to acc 444780672 bytes, to host 0 bytes)

ACC: Execute kernel main_$ck_L158_1 blocks:126 threads:128
                  async(auto) from himeno_F_v1.F90:158
ACC: Wait async(auto) from himeno_F_v1.F90:158

ACC: Start transfer 14 items from himeno_F_v1.F90:158
ACC:       free 'p' (34213896 bytes)

ACC:       copy to host, free 'wrk2' (34213896 bytes)

ACC:       copy to host, done reusable <internal> (8 bytes)
ACC:       done reusable <internal> (4 bytes)
ACC:       done reusable <internal> (0 bytes)
ACC: End transfer (to acc 0 bytes, to host 34213904 bytes)
```

Similar messages for a,b,c,bnd,wrk1

Similar messages for jmax,kmax,omega

Similar messages for a,b,c,bnd,wrk1, imax,jmax,kmax,omega

Runtime feedback: CRAY_ACC_DEBUG

```
ACC: Start transfer 14 items from himeno_F_v1.F90:158
ACC:       allocate, copy to acc 'p' (34213896 bytes)
ACC:       allocate
ACC:       allocate,

ACC:       allocate 
ACC:       allocate 
ACC:       allocate 
ACC: End transfer (t

ACC: Execute kernel 

ACC: Wait async(auto

ACC: Start transfer 
ACC:       free 'p' 

ACC:       copy to h

ACC:       copy to h
ACC:       done reus
ACC:       done reus
ACC: End transfer (t
```

Similar messages for

Bytes transfrd	variable	dirn	no. xfrs	mean size
14096125152	a	acc	103	136855584
10572093864	c	acc	103	102641688
10572093864	b	acc	103	102641688
3524031288	wrk2	host	103	34213896
3524031288	wrk1	acc	103	34213896
3524031288	p	acc	103	34213896
3524031288	bnd	acc	103	34213896
824	omega	acc	103	8
412	kmax	acc	103	4
412	jmax	acc	103	4
412	imax	acc	103	4

Total bytes transferred: 49336440092

A first data region

```
!$omp target data map(tofrom:p) &
!$omo             map(to:a,b,c,wrk1,bnd) &
!$omp             map(alloc:wrk2)
   iter_loop: DO loop = 1,nn

    gosa = 0d0

!$omp target teams distribute &
!$omp   reduction(+:gosa) private(s0,ss) map(from:wrk2)
<stencil: p(:,:,:) -> wrk2(:,:,:)>

!$omp target teams distribute
<copy: wrk2(:,:,:) -> p(:,:,:)>

   ENDDO iter_loop

!$omp end target data
```

~~3.3 Gflops~~

~~1.5 Gflops~~

27.0 Gflops

COMPUTE | STORE | ANALYZE

An outer data region

```
!$omp target data map(alloc:p,a,b,c,bnd,wrk1,wrk2)

CALL initmt ! initialisation
<two target regions>

CALL jacobi(nn,gosa) ! calibration
<two target regions, one data region>

cpu0 = gettime()
CALL jacobi(nn,gosa) ! performance
cpu1 = gettime()

!$omp end target data
```

~~3.3 Gflops~~
~~1.5 Gflops~~
~~27.0 Gflops~~
32.5 Gflops
(3x CPU)

An outer data region: performance feedback

```
Table 3:  Time and Bytes Transferred for Accelerator Regions

   Host | Host |  Acc | Acc Copy | Acc Copy | Events |Calltree
  Time% | Time | Time |       In |      Out |        | Thread=HIDE
        |      |      | (MBytes) | (MBytes) |        |

 100.0% | 0.01 | 0.01 |     0.00 |     0.00 |     34 |Total
|------------------------------------------------------------------------------
| 100.0% | 0.01 | 0.01 |     0.00 |     0.00 |     34 |main_
|        |      |      |          |          |        | main_.ACC_DATA_REGION@li.163
3  99.9% | 0.01 | 0.01 |     0.00 |     0.00 |     30 |  main_.ACC_REGION@li.163
||||---------
4|||  94.4% |
4|||   4.3% |
|============
```

```
Bytes transfrd              variable dirn   no. xfrs        mean size

           828                  kmax  acc        207               4
           828                  jmax  acc        207               4
           828                  imax  acc        207               4
           824                 omega  acc        103               8

Total bytes transferred:  3308
```

NekBone

EPiGRAM Project

3 years to Oct.16

www.epigram-project.eu

EPiGRAM

6 partners

€3M

KTH (SE)

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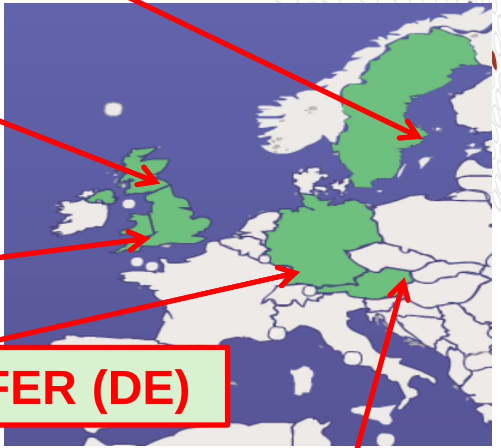
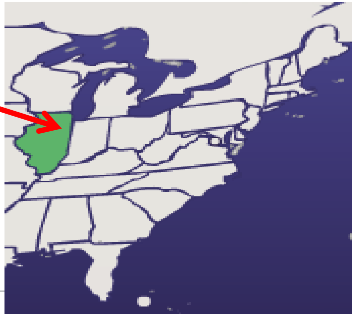


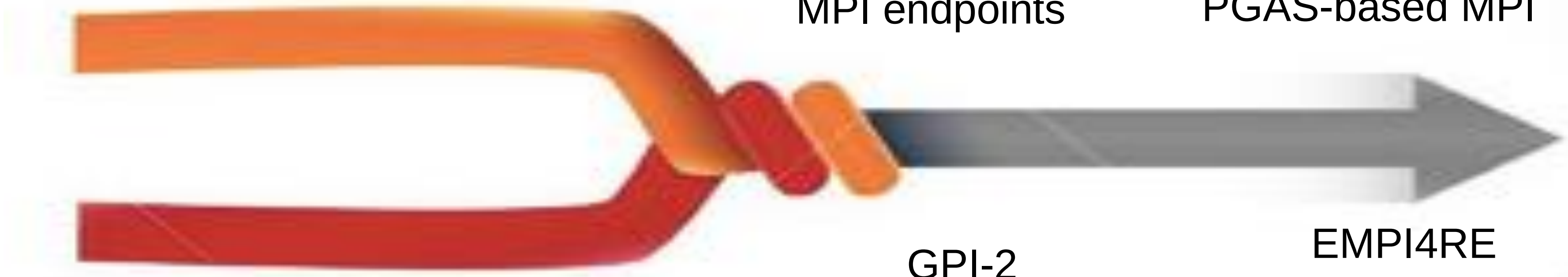
UIUC (USA)



CREST

EPiGRAM Integrated Vision

MPI:
- Persistent Collectives
- Neighborhood collectives



MPI endpoints

PGAS-based MPI

GPI-2:
- Fast RDMA; Fault-tolerance

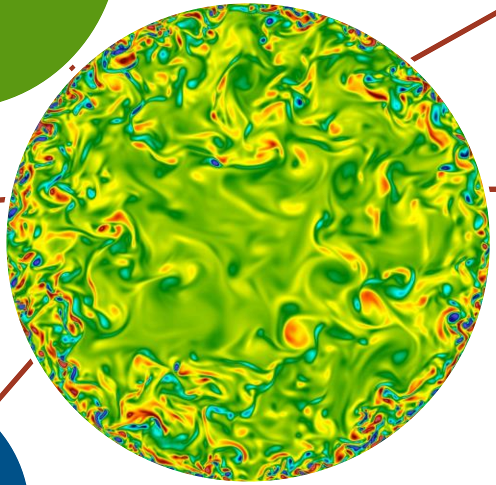
Diverse memory spaces:
- OpenACC, OpenMP, …

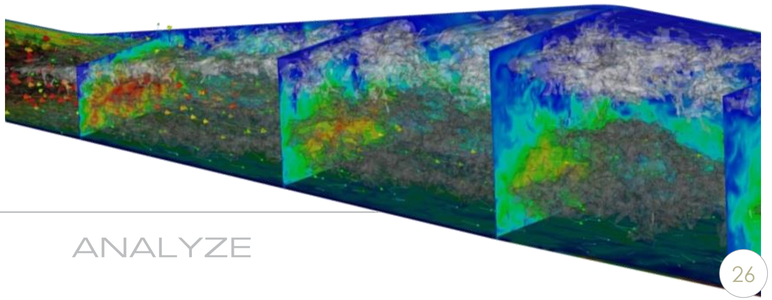
GPI-2
Isolation of library

EMPI4RE
EPiGRAM MPI for
RESEARCH

Nek5000

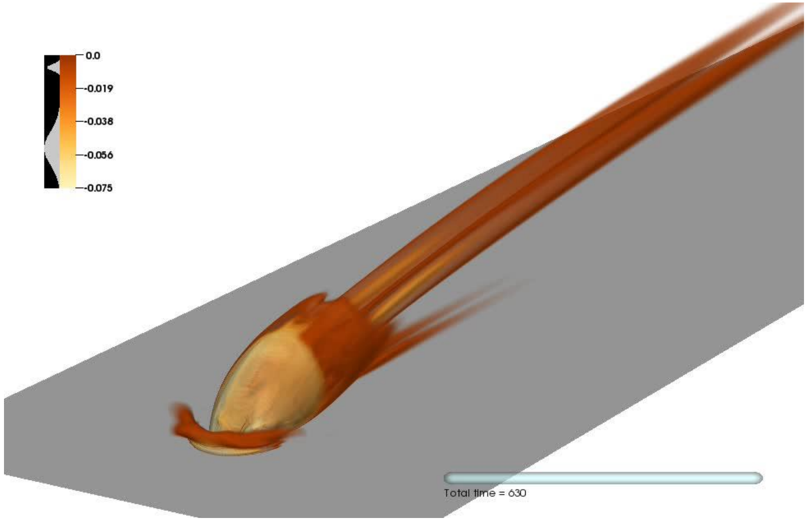
- astrophysics
- combustion
- reactor core
- oceanography
- vascular flow





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
  - EPiGRAM simplified comms



Nek5000 simulation of a cross-flow on a flat panel

NekBone

- **Small testcase, for functionality/quick development**
  - Elements per PE: Nelt=32
  - Spectral order: N=10
- **Computational load:**
  - Multiple (Nelt), small (NxN) matrix-matrix multiplications
- **Configuration:**
  - 8 nodes, one MPI rank per node (no OpenMP threading)
- **Code reports performance (and correctness)**
  - Intel IVB CPU: 40.2 GFlops

Nekbone porting

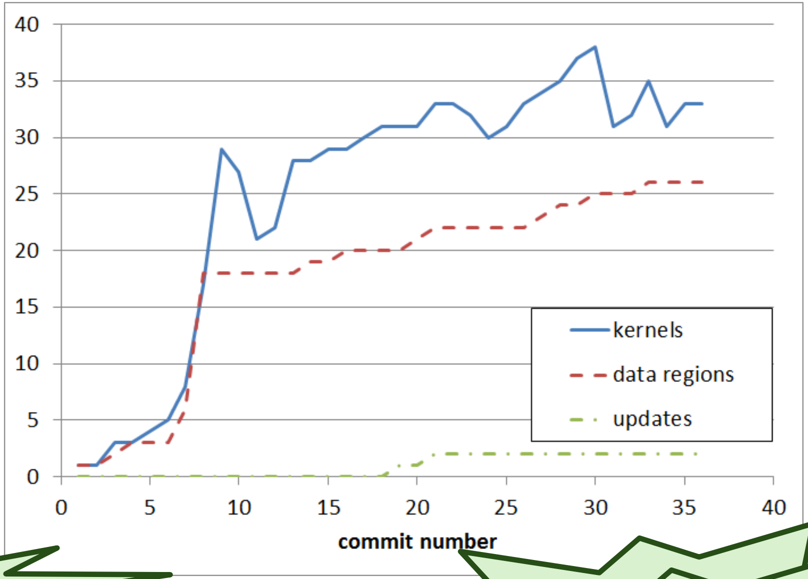
- **Proceeds in same way as for Himeno**
  - Code already has performance counters and correctness checks
  - Profile to understand the hotspots, calltree and loopnests
  - Begin with target regions on leaf nodes
  - Expand data regions up the calltree

- **Parallel ports: OpenMP device constructs; OpenACC**
  - Maintained audit trail in git log:
    - Correctness, directive count, performance, rough profile

How many directives?

OpenMP

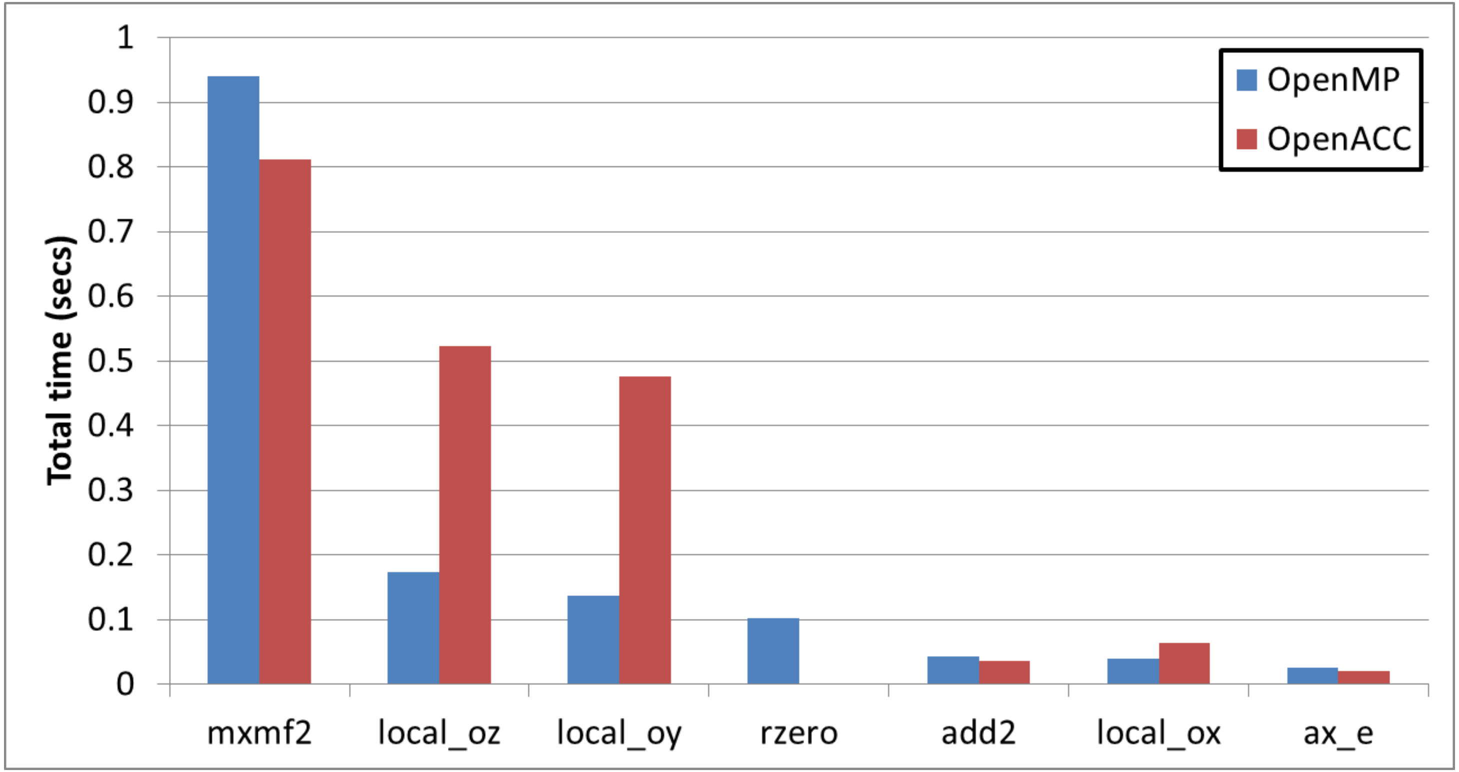
OpenACC



420 Mflops

G2G MPI

Performance of NekBone kernels



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
```

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----------->
```

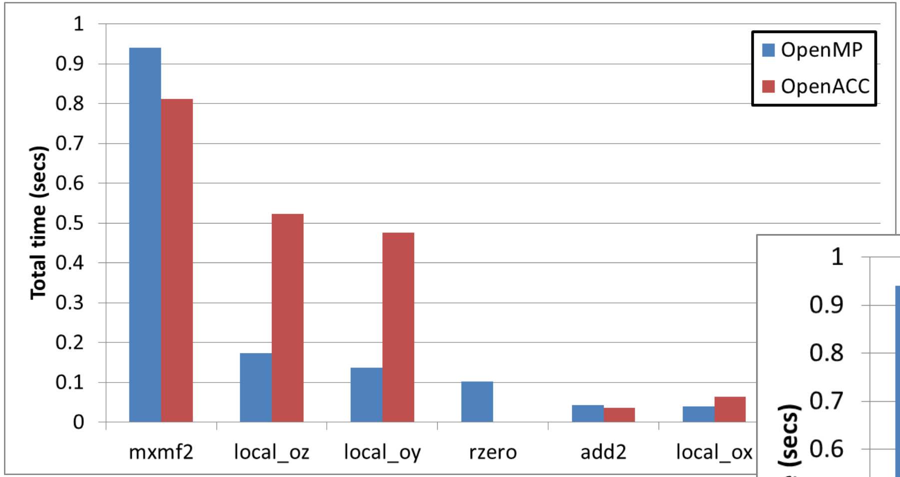
863µs→147µs

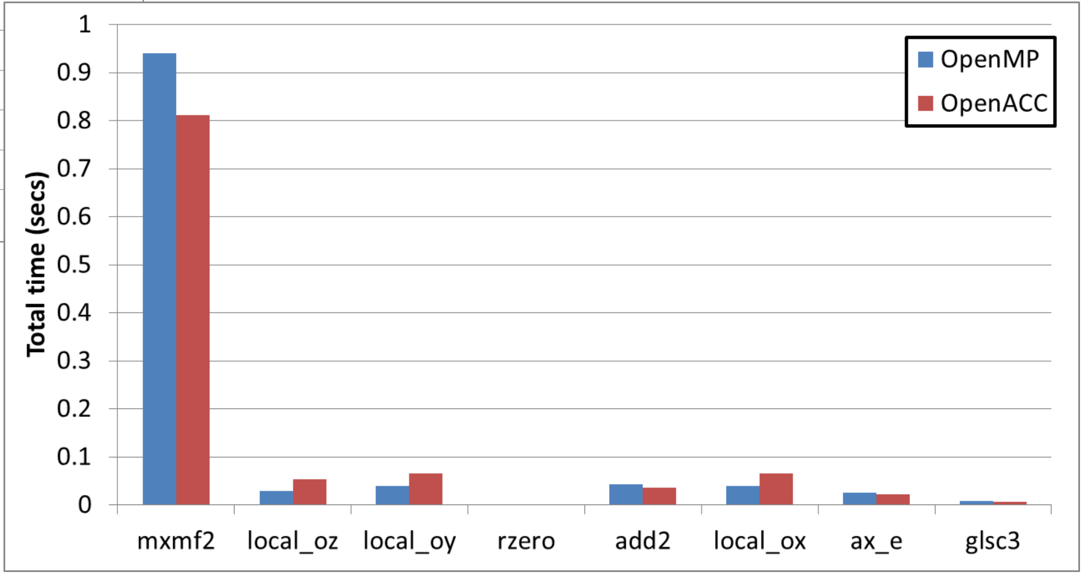
```
G-----------< !$acc parallel loop

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 5--<     do i=1,n_shared
G C C g 5         w(l_face_z_back(i),e_back)= &
G C C g 5            w(l_face_z_back(i),e_back)+ &
G C C g 5            w(l_face_z_front(i),e_front)
G C C g 5         w(l_face_z_front(i),e_front) = &
G C C g 5            w(l_face_z_back(i),e_back)
G C C g 5-->     enddo
G C C g----->   enddo
G C C------->  enddo
G C---------> enddo
G----------->
```

2592µs→261µs

Performance after tuning





Conclusions

- **Directives offer productive performance-portability**
  - NekBone: 1 directive per 160 lines of code
- **OpenMP device constructs are mature prog. model**
  - v4.0 offers rich feature set; more coming v4.1
- **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**

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