# The Broader Picture of Using Accelerator Directives in Your Code

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Third Workshop on Accelerator Programming Using Directives

OAK RIDGE National Laboratory | OAK RIDGE LEADERSHIP COMPUTING FACILITY

SC16 Salt Lake City, Utah | hpc matters.

# My Background

- Computational Climate Science
  - Liaise with INCITE projects running on OLCF machines
  - Accelerated Model for Climate and Energy
- Center for Accelerated Application Readiness
  - Funded by OLCF
  - Prepared codes for Titan before it arrived
  - Currently preparing codes for Summit before it arrives
- Fluids algorithm development for modern HPC

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  - Same code cannot run on GPU and CPU
  - Gradual porting not really possible
    - Detecting bugs significantly more difficult
  - Optimized code looks nothing like the original code
    - Difficult to merge CPU code changes into CUDA
    - Scientific programmers cannot understand it
    - Unmaintainable and unportable

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  - Accelerated and CPU code must look similar
- Easier debugging: run same code on CPU and accelerator

# Other Options

- Templated C++ → “kokkos”
  - However, you have to marry it and stick with it
- “Domain Specific Languages”
  - Are they just glorified if-statements?
  - Ad-hoc to the application in question
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- Directives offer greater flexibility

# Refactoring: Relatively Little Work Per Node

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!$omp parallel do
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 do k = 1 , nlevels
  mass(k,ie) = sum(vals(:,:,k,ie))
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- Must refactor the code

```
call memset( mass , 0 )
!$acc parallel do collapse(4)
do ie = 1 , nelements
 do k = 1 , nlevels
  do j = 1 , ny
   do i = 1 , nx
    masstmp = mass(k,ie)
    valtmp = vals(i,j,k,ie)
    !$acc atomic update
    masstmp = masstmp + valtmp
```

# Refactoring: Low-Level Calls w/ Too Little Work

- Good SE practices → reusable low-level routines

```
do ie = 1 , nelements
 do k = 1 , nlevels
  grad = gradient(dat(:,k,ie))
 enddo
enddo

function gradient(dat) result(r)
 r = matmul( grad_mat , dat )
end function gradient
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do ie = 1 , nelements
 do kc = 1 , kchunk
  grad = gradient(dat(:,:,ie),kc)
 enddo
enddo

function gradient(dat,kc) result(r)
 do kk = 1 , kchunk
  do i = 1 , n
   k = (kc-1)*kchunk + kk
   tmp = 0
   do m = 1 , n
    tmp = tmp + grad_mat(i,m)*dat(m)
   enddo
   r(i,k) = tmp
  enddo
end function gradient
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- Stop using "matmul"

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  - Poorly-sized inner loop dimension (vectorization)
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- Indirect addressing on fastest-varying dimension
  - Doesn’t saturate wide memory bus;  Doesn’t vectorize efficiently
  - Best to pad indirect addressing with contiguous dimension

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**Much of accelerator refactoring benefits the CPU**

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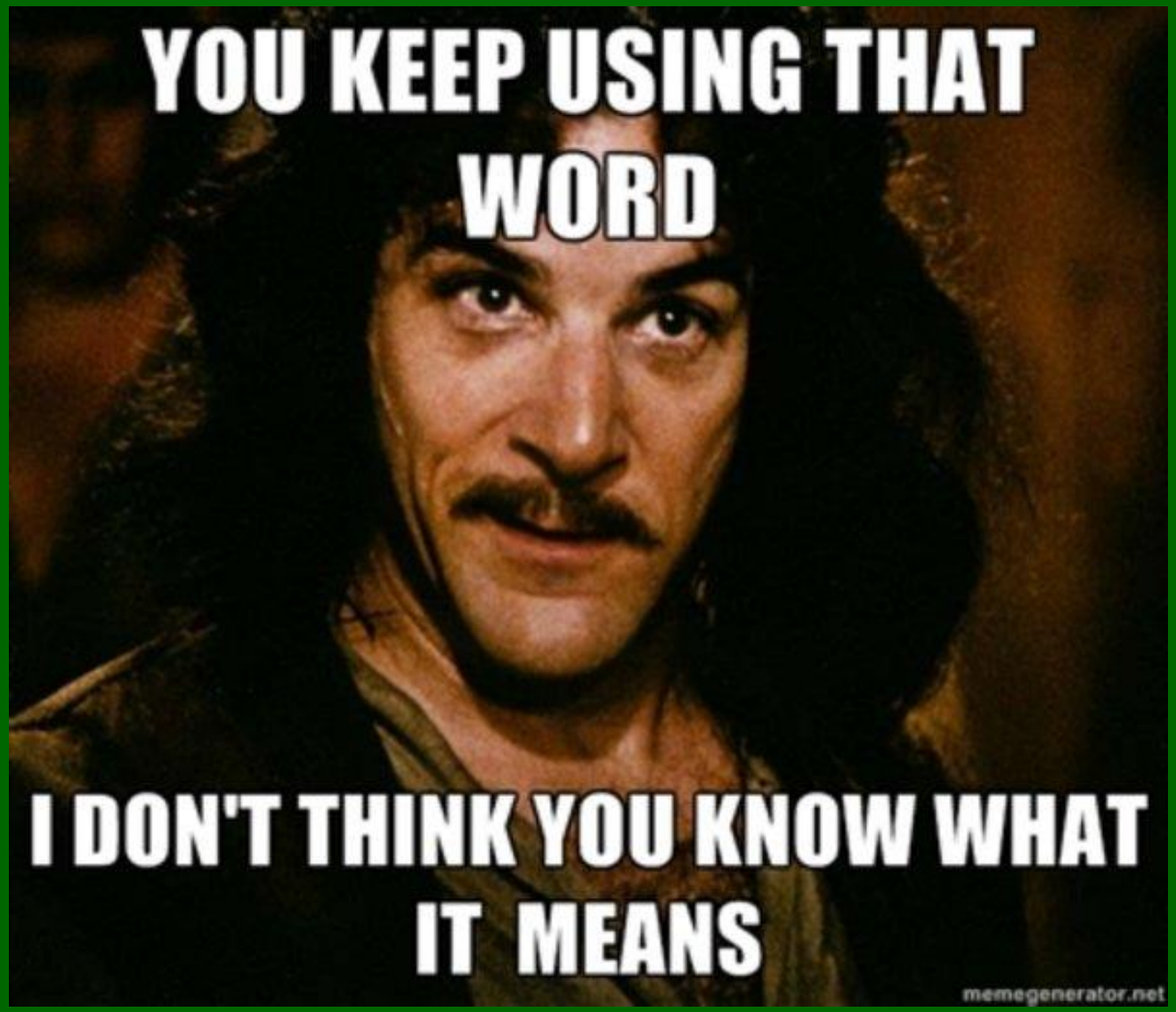

# “Performance Portability”

- Identical code will never perform optimally on all platforms
  - CPU vector length: 256 bits (8 “vector threads”)
    - Heavily cache-based
  - KNL vector length: 512 bits  x  2 (16-32 “vector threads”)
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- Directives inherently balance performance & maintainability
- Often best to branch the code, but at the lowest level possible
- Similar looking code is easier to maintain

# Things That Can Help Performance Portability

- CPU's / MIC's being able to handle if-statements in vector units
- The ability to use nested "omp do" and "acc loop" in the same vector / thread context
- GPUs fixing their "register explosion" problem with long kernels
- CPU's & MIC's allowing users to prioritize / specify data for cache
- All compilers implementing automatic directive-based tiling
- GPU implementations improve performance of manually strip-mined loops (as opposed to having to be collapsed)

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- A feature you rely on heavily that isn’t supported is a bug

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- Be kind: Compiler developers are people too

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- OpenMP and OpenACC are as much sociology as technical
  - App. Developer: “I won’t use it because it isn’t mature.”
  - Compiler Developer: “It immature because you won’t use it.”
- You determine when it’s appropriate to try things out
  - But “mature” is not a well-defined idea
  - Accelerator directives will always have room for improvement

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**We <u>all</u> benefit when you engage compiler developers**

**https://developer.nvidia.com/accelerated-computing-developer**

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 tmp2 = routine2(tmp1)
 [Intermittent work]
 data3(:,:,ie) = routine3(tmp1,tmp2)
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- Have to break up loops and turn local temps into globals

```
do ie = 1 , nelements
 glob1(:,:,ie) = &
                 routine1(data1(:,:,ie))
 [Intermittent work]
enddo
do ie = 1 , nelements
 glob2(:,:,ie) = &
                 routine2(glob1(:,:,ie))
 [Intermittent work]
enddo
do ie = 1 , nelements
 data3(:,:,ie) =  &
               routine3(glob1(:,:,ie),&
                        glob2(:,:,ie))
enddo
```