NERSC8 CoE
Key Actions when optimizing for KNL

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Outline

- **Characterization and Multi-node Considerations**
  - Target Science
  - Profiles and Hotspots
  - Scaling and Communication
- **Single node optimizations**
  - Memory and cache footprint analysis
  - Memory bandwidth requirements
  - Vectorization
  - Creating a kernel to aid in further analysis and testing
- **Example: BerkeleyGW - FF kernel**

What Science do you want to run on Cori

- **Identify 1 or a few science problems that you anticipate running on Cori**
  - Identifying the science problems will help focus efforts on what routines and issues are important
- **Estimate how many nodes you will use during the run**
  - Does the code already scale this high?
  - What can we say about communication
- **The combination of science problem and number of nodes will allow one to estimate memory footprints, array sizes, and trip count sizes**
  - This information is critical

Scaling and communication

- **How high does the code scale**
- **Does your code use both OpenMP and MPI?**
  - How many OpenMP threads can you utilize
- **What is limiting your scaling?**
  - Communication overhead?
  - Lack of parallelism on a given science problem
- **Understand and optimizing scaling is critical**
  - KNL requires scaling to higher numbers of cores to achieve the same level of performance
  - Scaling impacts loop trip counts, memory footprints, and more

Where is the time being spent

- **Are you sure? Verify**
- **Use statistical profilers to determine where the time is being spent**
  - Are there obvious key routines that time up a significant percentage of time?
  - Are there key loops or code sections?
  - How many routines before you hit 80% of the run time
- **Is the profile different for different science problems?**

Understanding your memory footprint is critical

- **Do you expect to your problem to consume a significant amount of main memory?**
  - Main memory is about 96 Gbytes
- **Is it possible that your problem will fit into fast memory**
  - Fast memory is 16 Gbytes per node
    - Can be configured as a “memory cache”
    - Can be configured 50% cache and 50% explicitly managed
    - Can be configured 25% cache and 75% explicitly managed
    - Can be configured at 100% explicitly managed
- **What is the memory access pattern for the routines and loops identified as important**
  - What are the trip counts in that loop nest?
  - How much data is accessed?
  - How much is reused more than once?

Vectorization

- **Do the loops vectorize?**

- **Vectorization is very important to achieving high performance rates**
  - Edison vectors are 4 DP words, Cori is longer
  - Cannot take full advantage of functional units without vectorization
  - Unlikely to take full advantage of memory bandwidth
  - Scalar performance on Cori

- **Common inhibitors**
  - Dependencies
  - Indirect addressing may prevent vectorization or make is less efficient
    - e.g. A(indx(i)) =
  - Function / subroutine calls
  - If tests inside of inner loops may slow execution and prevent vectorization
  - More…

Are your kernels memory bandwidth bound

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How can you tell if you are memory bandwidth bound?

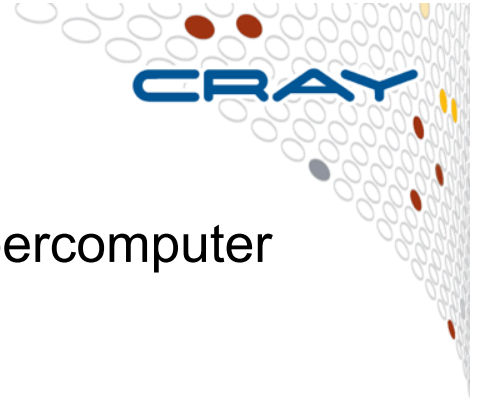
- **Sometimes it is easy**
  - One or more loop nests are streaming through a huge amount of data
  - Little to no reuse
  - Easy to determine the
- **Sometimes it is difficult**
  - Some trip counts are large
  - But some data are reused
  - Not obvious what the compiler did
  - Not obvious if the data remains in cache
- **Counters can be difficult to interpret**
  - Difficult to keep track of different levels of cache

- **Try to run kernel using 1 or 2 fewer cores**
  - Adjust the number of OMP threads
  - Use aprun –S option to spread mpi ranks across more sockets
  - If performance per socket does not change, kernel may be bandwidth bound
- **Try and examine trip counts and reference patterns**

Create kernel that are representative of critical loops

- **Use all of the information previously discussed to create kernels to be used for further investigation**
- **Trip counts and array sizes per node should be as accurate as possible**
  - Goal is to reflect what are real science problem running on a significant portion of the machine would look like on a single socket
- **Kernel should use all of the cores of a single socket on Edison**
  - Kernels that only run on a single core will not capture the full memory footprint and bandwidth characteristics of the real code

Why do we need a kernel?



- **Extreme flexibility and portability**
  - Cannot assume we will always run on a multi-node supercomputer
  - Might not even run it “directly” on a computer
- **Run on many different platforms**
  - Single socket of edison
  - KNC whitebox
  - KNL simulator or emulator
  - Early KNL hardware
  - KNL whitebox
- **Focused analysis**
  - Some tools may not be able to run a full program
  - Want to focus on a particularly important area
- **Flexible experimentation**
  - Try different compilers and options without porting entire code
  - May want to try different “decompositions” and optimizations that would (temporarily) break the larger code

Example Analysis and Optimizations:

BerkeleyGW

BerkeleyGW

- **Identified 4-6 kernels**
  - GPP
  - FF
  - BSE
  - Chi Summation
  - FFT (library not analyzed by Cray)
  - Scalapack (library not analyzed by Cray)

- **Cray analyzed and provided potential optimizations GPP, FF, BSE, and Chi Summation for:**
  - Vectorization
  - Memory footprint requirements
  - Memory bandwidth requirements
  - OpenMP effectiveness
  - Cray and Intel compiler

- **Next few slides review some of the work done for FF**

BerkeleyGW kernels: FF

- **Excellent vectorization and OpenMP**
- **Used craypat to examine where time was being spent**

```
module unload darshan  # darshan does not seem to play well with craypat
module load perftools
ftn -rm -o ffkernel.x ffkernel.f90
pat_build ffkernel.x
run
pat_report ffkernel.x+pat+36422-5701s.xf > ffkernel.manyfreq.patreport
```

- **Generates both a routine level…**

```
 100.0% | 585.0 |   -- |    -- |Total
|-----------------------------------------------
|  81.9% | 479.0 |   -- |    -- |USER
||----------------------------------------------
||  64.4% | 377.0 | 10.8 |  3.1% |ffkernel_.LOOP@li.388
||  12.6% |  74.0 |   -- |    -- |ffkernel_
||   3.8% |  22.0 |  4.2 | 19.3% |ffkernel_.LOOP@li.517
```

- **… and a line level statistical profile report**

```
||  64.4% | 377.0 |   -- |    -- |ffkernel_.LOOP@li.388
||||-------------------------------------------------------
4|||  25.6% | 150.0 | 29.6 | 18.8% |line.406
4|||  12.5% |  73.0 | 11.2 | 12.7% |line.408
4|||  25.1% | 147.0 | 14.0 | 10.1% |line.414
```

BerkeleyGW kernels: FF

- **Line level statistical profile report**

```
||   64.4% | 377.0 |   -- |    -- |ffkernel_.LOOP@li.388
||||-------------------------------------------------------------------
4|||  25.6% | 150.0 | 29.6 | 18.8% |line.406
4|||  12.5% |  73.0 | 11.2 | 12.7% |line.408
4|||  25.1% | 147.0 | 14.0 | 10.1% |line.414
```

```
!$OMP PARALLEL do private (my_igp,igp,indigp,igmax,ig,schDtt,I_epsRggp_int, &
!$OMP I_epsAggp_int,schD,schDt,ifreq) reduction(+:schdt_array)     !This was line 388 in the source
do ifreq=1,nFreq
  do my_igp = 1, ngpown
    do ig = 1, igmax
      I_epsRggp_int = I_epsR(ig,my_igp,ifreq)   !This was line 406 in the source
      I_epsAggp_int = I_epsA(ig,my_igp,ifreq)   !This was line 408 in the source
      schD=I_epsRggp_int-I_epsAggp_int
      schDtt = schDtt + matngmat(ig,my_igp)*schD  !This was line 414 in the source
    enddo
  enddo
enddo
```

- **Don’t focus too much on the time spent in one line vs another…**
- **…The point is that it is clear that a very significant amount of time is being spent in this loop nest / region**

BerkeleyGW kernels: FF

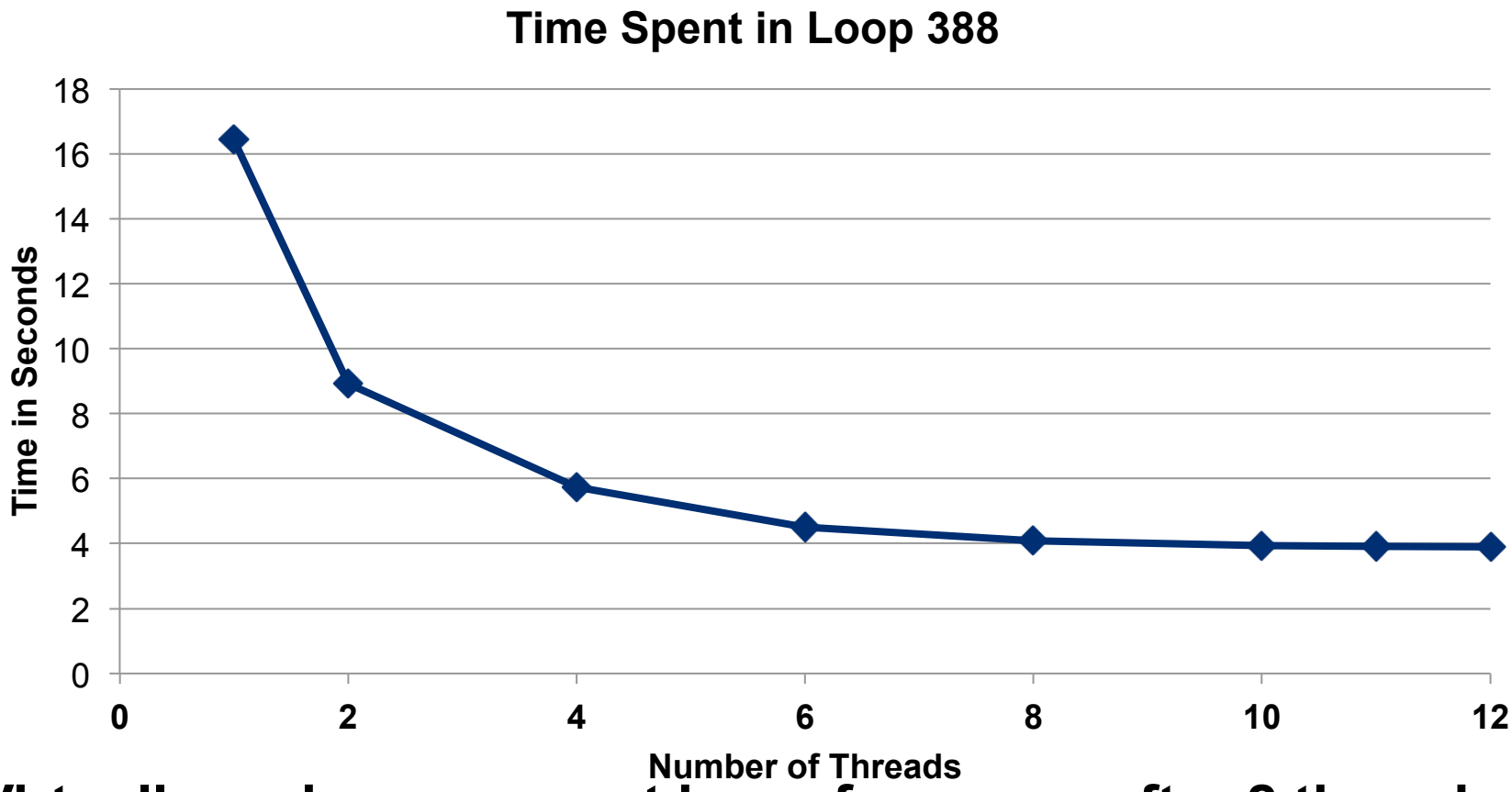
- **Examined trip counts and declarations to calculate memory footprint and reuse**
  - nFreq = 20000
  - Ngpown = 20
  - Igmax = 1000

```
!$OMP PARALLEL do private (…  &
!$OMP …) reduction(+:schdt_array)
do ifreq=1,nFreq
  do my_igp = 1, ngpown
    do ig = 1, igmax
      I_epsRggp_int = I_epsR(ig,my_igp,ifreq)
      I_epsAggp_int = I_epsA(ig,my_igp,ifreq)
      schD=I_epsRggp_int-I_epsAggp_int
      schDtt = schDtt + matngmat(ig,my_igp)*schD
    enddo
  enddo
enddo
```

- **Lots and lots of parallelism**
- **I_epsR and I_epsA were each about 1.6 Gbytes with no immediate reuse**
- **matngmat about 80 kbytes, and shared across threads**

BerkeleyGW kernels: FF

- Let's examine OpenMP scaling for a moment



- Virtually no improvement in performance after 8 threads
- Yet we know there is lots and lots of parallelism

BerkeleyGW kernels: FF

- **Streaming data arrays that are more than 3 Gbytes in size**
- **Lots of parallelism, but performance stops improving**

- **Conclusion: Loop was memory bandwidth bound**

- **On Cori I_epsR might fit into fast memory**
  - But then we would still just be limited by the bandwidth of fast memory
- **Only way to go faster is to find more data reuse**

```
do ifreq=1,nFreq
  do my_igp = 1, ngpown
    do ig = 1, igmax
      I_epsRggp_int = I_epsR(ig,my_igp,ifreq)
      I_epsAggp_int = I_epsA(ig,my_igp,ifreq)
      schD=I_epsRggp_int-I_epsAggp_int
      schDtt = schDtt + matngmat(ig,my_igp)*schD
    enddo
  enddo
enddo
```

BerkeleyGW kernels: FF

- **Realized there was a "nbands" loop at a relatively high level that reused the I_eps* variables**
  - Worked to effectively cache block main loops

```
do ifreq=1,nFreq
  do igbeg = 1,igmax,igblk
    igend = min(igbeg+igblk-1,igmax)
    do my_igp_beg = 1, ngpown,cblk
      my_igp_end = min(my_igp_beg+cblk-1,ngpown)
      do n1_beg=1,number_bands,cblk
        n1_end = min(n1_beg+cblk-1,number_bands)
        do my_igp = my_igp_beg,my_igp_end
          do n1=n1_beg,n1_end
            …
            do ig = igbeg, igend
              I_epsRggp_int = I_epsR(ig,my_igp,ifreq)
              I_epsAggp_int = I_epsA(ig,my_igp,ifreq)
              schD=I_epsRggp_int-I_epsAggp_int
              schDtt=schDtt+aqsntemp(ig,n1) *CONJG(aqsmtemp(igp,n1))*schD
            enddo
            schdt_matrix(ifreq,n1) = schdt_matrix(ifreq,n1) + schDtt
          enddo
        enddo
      enddo
    enddo
  enddo
enddo
```

I_eps arrays do not change with n1

- **Resulted in a 4X improvement in wall-clock time on XEON**

BerkeleyGW kernels: FF

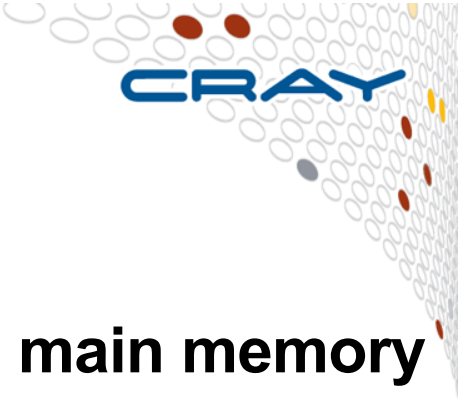
- **Realized there was a "nbands" loop at a relatively high level that reused the I_eps* variables**
  - Worked to effectively cache block main loops

```
do ifreq=1,nFreq
  do igbeg = 1,igmax,igblk
    igend = min(igbeg+igblk-1,igmax)
    do my_igp_beg = 1, ngpown,cblk
      my_igp_end = min(my_igp_beg+cblk-1,ngpown)
      do n1_beg=1,number_bands,cblk
        n1_end = min(n1_beg+cblk-1,number_bands)
        do my_igp = my_igp_beg,my_igp_end
          do n1=n1_beg,n1_end
            …
            do ig = igbeg, igend
              I_epsRggp_int = I_epsR(ig,my_igp,ifreq)
              I_epsAggp_int = I_epsA(ig,my_igp,ifreq)
              schD=I_epsRggp_int-I_epsAggp_int
              schDtt=schDtt+aqsntemp(ig,n1) *CONJG(aqsmtemp(igp,n1))*schD
            enddo
            schdt_matrix(ifreq,n1) = schdt_matrix(ifreq,n1) + schDtt
          enddo
        enddo
      enddo
    enddo
  enddo
enddo
```

aqsntemp array does not change with my_igp

- **Resulted in a 4X improvement in wall-clock time on XEON**

Data Reuse will be important



- Data reuse will be critical to performance
- Reuse out of HBM will reduce requirements on main memory
- Reuse out of lower levels of cache will lower requirements on HBM
- In order to know how to cache block properly we need to know the trip counts of loops and the sizes of various arrays as accurately as possible

Summary

- **Code Characterization will be an important first step in preparing for Cori**
  - Target Science
  - Target Scaling
  - Hotspot identification
- **Cori node is different from Edison node**
  - Single node optimizations will be an early focus
  - A properly designed kernel will help with optimization efforts
  - Vectorization will be more important in the future
- **Data reuse will be important, but how important will depend on memory footprints and access patterns**