ICHEC
Irish Centre for High-End Computing

Benefits and Costs of Coarse-Grained Multithreading for HARMONIE

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sfi Science Foundation Ireland
Ireland's EU Structural Funds Programmes 2007 - 2013
Co-funded by the Irish Government and the European Union
EUROPEAN REGIONAL DEVELOPMENT FUND
AN ROINN OIDEACHAIS AGUS EOLAIOCHTA | DEPARTMENT OF EDUCATION AND SCIENCE
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Executive Summary

In the future (present?) ever more parallelism will be needed:

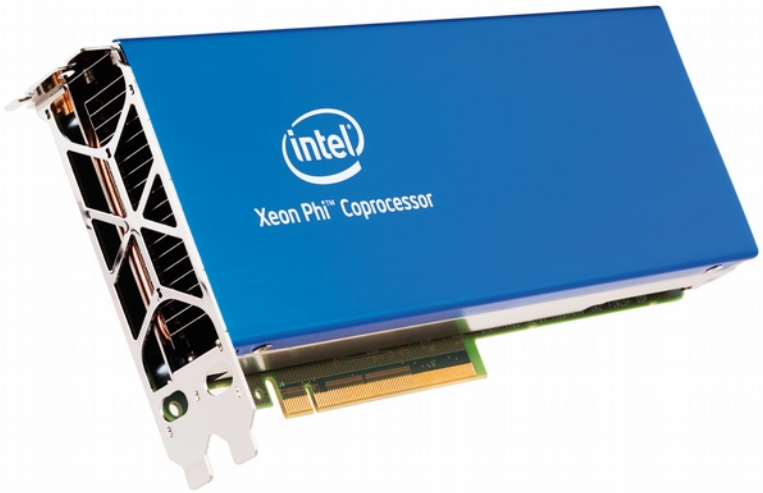
1. MPI for inter-node parallelism
2. OpenMP multithreading for intra-node parallelism
3. Vectorization for intra-core parallelism

There will be no escape from multithreading:

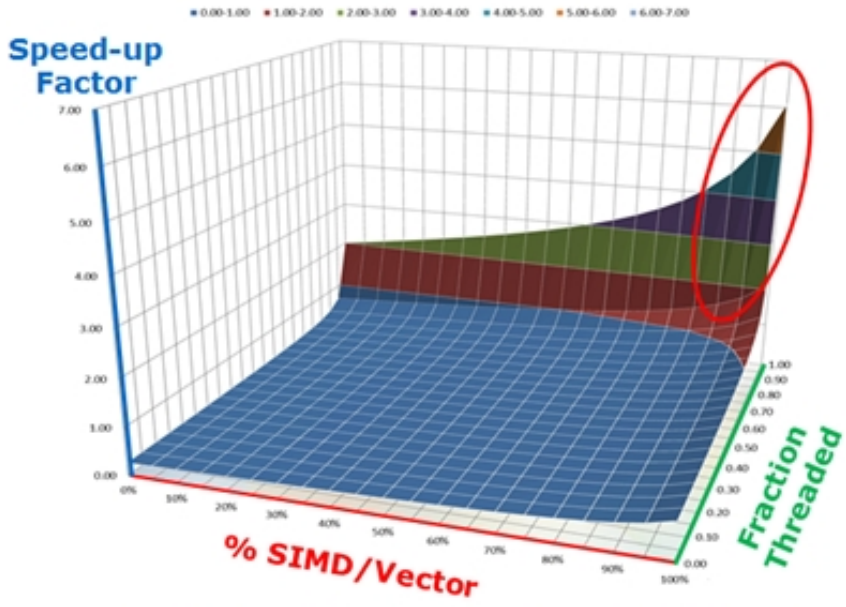
- MPI-only will not scale to (#nodes x #cores/node)
  - MPI_alltoall would excessively dominate run-time.
- HARMONIE already has quite "coarse-grained" multithreading…
  - But it is still not "good enough".
  - Could it be even more fully "coarse-grained"?
  - Is full OpenMP domain decomp. (like MPI) possible, or desirable?
- Cycle 40 looks like it makes much better use of OpenMP.

Motivation

- The mission: make HARMONIE work on Xeon Phi coprocessors.
- HARMONIE now runs on Xeon Phi, in “native”, “symmetric”, and even “offload” mode – but only very slowly.
- The problems are mostly with Xeon Phi*.
- But one issue we can address is the *multithreading in HARMONIE.*



*(See 2014 ASM presentation)



"Fine-Grained" vs. "Coarse-Grained" Multithreading

Fine-grained:

- Parallel regions created and destroyed multiple times during run.
- Each thread does relatively little work
- Parallel regions interspersed with sequential ones.
- Often loop-level parallelism, low in call-tree.

Coarse-grained:

- Parallel regions survive for long periods – even entire run.
- Each thread does a lot of work.
- Parallel regions interrupted by "critical sections"
- Domain-level parallelism, high in call tree.

Currently, HARMONIE has "partial" coarse-grained multithreading: it's at a high level in call-tree, but avoids true "subdomain decomposition".

Towards Full "Coarse-Grained" Multithreading

Consider a "global" domain of grid-points:

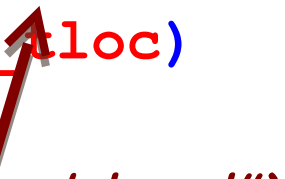
```
(NX_glob, NY_glob, NZ_glob)
```

After MPI decomposition, each MPI process sees:

```
(NX_loc,  NY_loc,  NZ_loc)
```

After more decomposition for coarse-grained multithreading:

```
(NX_loc,  NY_loc,  NZ_tloc)
```



("Thread-local")

Fine-Grained Multithreading Code

```
!$OMP PARALLEL DO PRIVATE(i,j,k)
      do k=2,nz_loc-1
        do j=2,ny_loc-1
          do i=2,nx_loc-1
            arr_out(i,j,k) = wght1*arr_in(i,j,k) + wght2*(
     &          arr_in(i-1,j,k) + arr_in(i+1,j,k) +
     &          arr_in(i,j-1,k) + arr_in(i,j+1,k) +
     &          arr_in(i,j,k-1) + arr_in(i,j,k+1) )
          enddo
        enddo
      enddo
!$OMP END PARALLEL DO
```

Partial Coarse-Grained Multithreading

```
!$OMP PARALLEL PRIVATE( <long list of private variables here...>)
 ...
   !$OMP SINGLE ! Only 1 thread does any I/O needed
      ...
   !$OMP END SINGLE
...
do icount=1,ncount  ! Main outer loop
    call halo_exchange(array,myrank,nx_loc,...) ! Critical sections?
    ...
   !$OMP DO
    do k=2,nz_loc+1  ! Central nested loops as in fine-grain case
        ...
    end do
   !$OMP END DO
 end do             ! End of main outer loop
!$OMP END PARALLEL
```

Full Coarse-Grained Multithreading

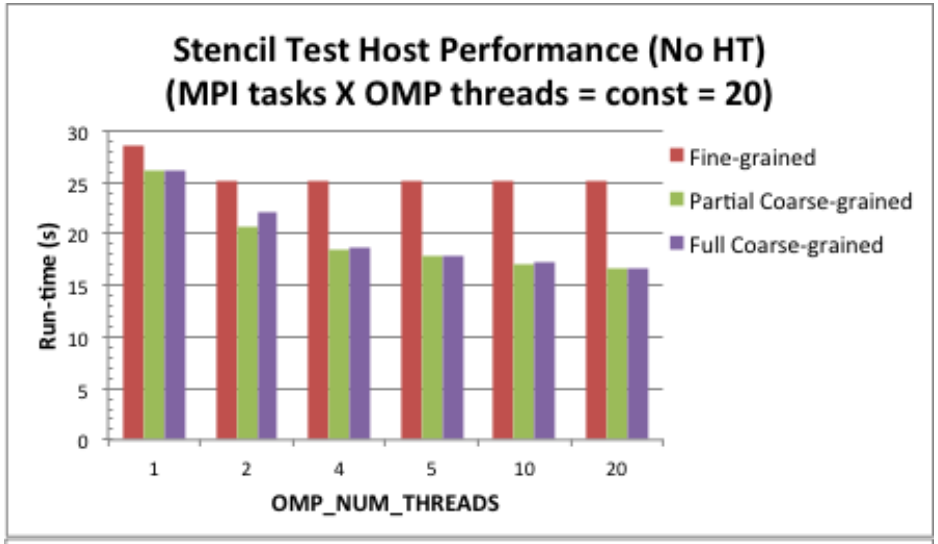
```
!!!real shado_E(ny_loc,nz_loc)   ! MPI-local
   real shado_E(ny_loc,nz_tloc) ! Thread-local
...
! Thread-wise decomposition needs extra book-keeping:
   kmin = mythread*nz_tloc ! For thread-local point range
...
! Extract the "shadow-zone" part of main array:
!!!!$OMP DO
!!!   do k=2,nz_loc +1    ! MPI-only
      do k=2,nz_tloc+1    ! Thread decomposition
          do j=2,ny_loc+1
!!!         shado_E(j-1,k-1) = ext_in(nx_loc+1,j,     k)
            shado_E(j-1,k-1) = ext_in(nx_loc+1,j,kmin+k)
          enddo
        enddo
!!!!$OMP END DO
```

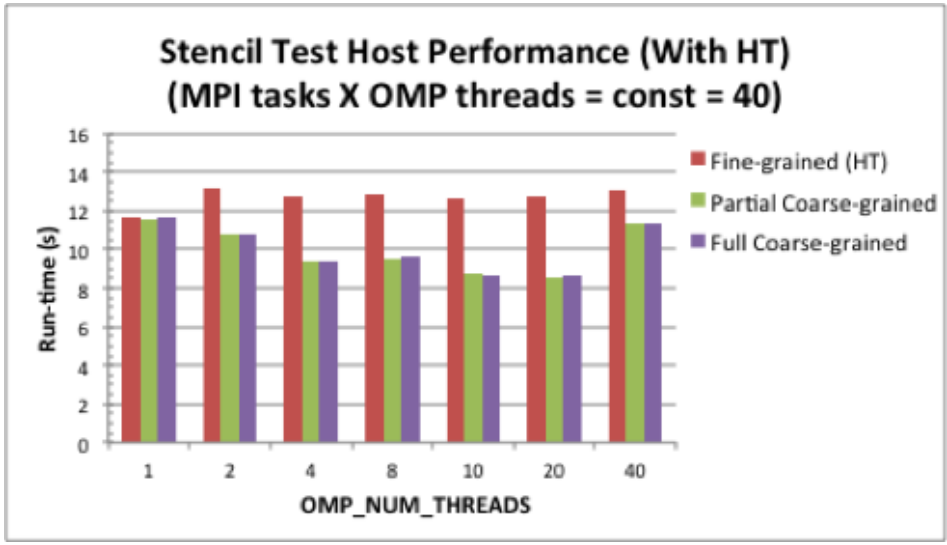
Full Coarse-Grained Multithreading, contd.

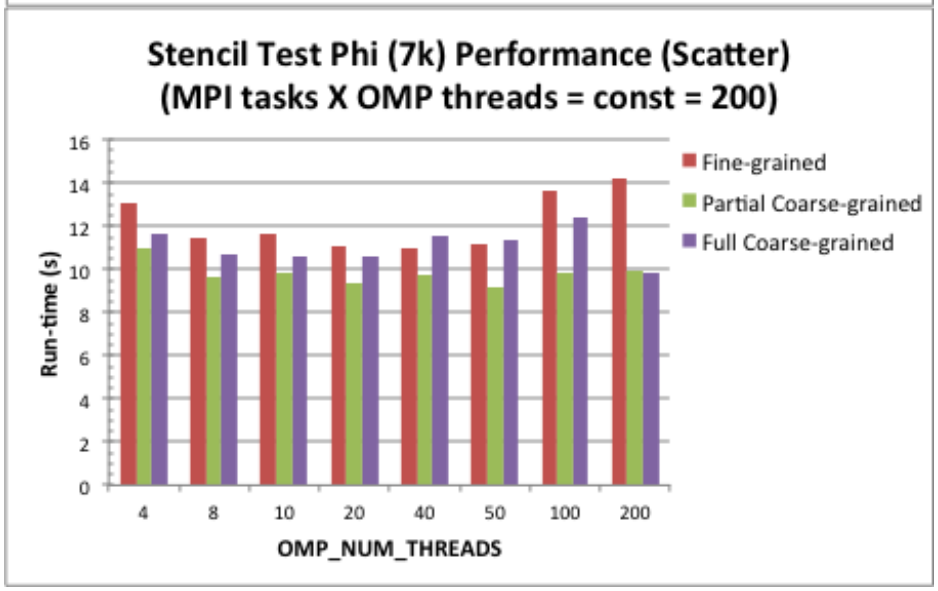
```
!!!!$OMP SINGLE
!Use if MPI not thread-safe: !$OMP ORDERED
!!! call MPI_Recv(shado_W(1,1),ny_loc*nz_loc ,MPI_REAL, &
    call MPI_Recv(shado_W(1,1),ny_loc*nz_tloc,MPI_REAL, &
  &      idest_e,itag_w,MPI_COMM_WORLD,istatus,ierror)
!
!!! call MPI_Send(shado_E(1,1),ny_loc*nz_loc, MPI_REAL, &
    call MPI_Send(shado_E(1,1),ny_loc*nz_tloc,MPI_REAL, &
  &      idest_e,itag_e,MPI_COMM_WORLD,ierror)
!Use this if MPI not thread-safe:    !$OMP END ORDERED
!!!!$OMP END SINGLE
```

Each thread now sends & receives its own messages - is this wise?

Coarse vs. Fine-grained OpenMP Parallelism



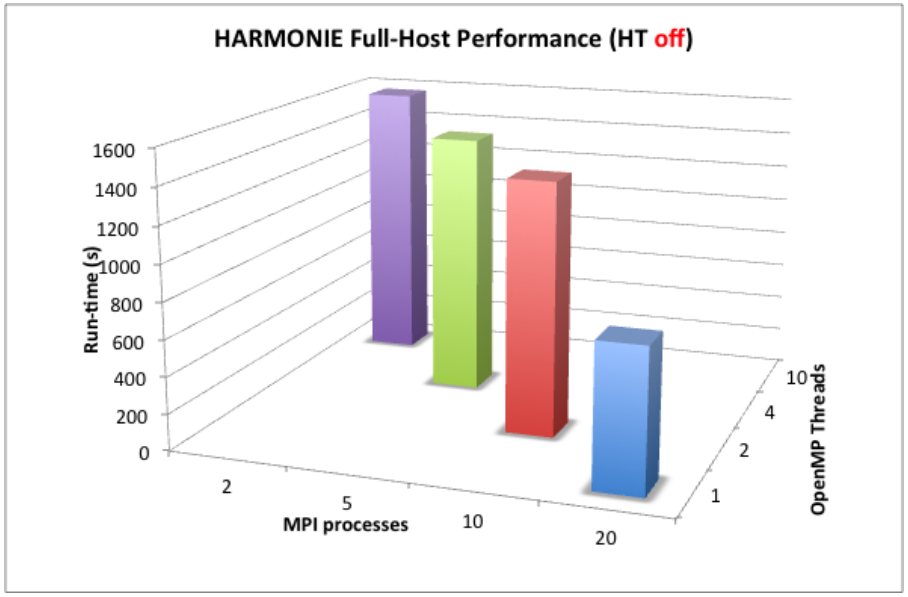




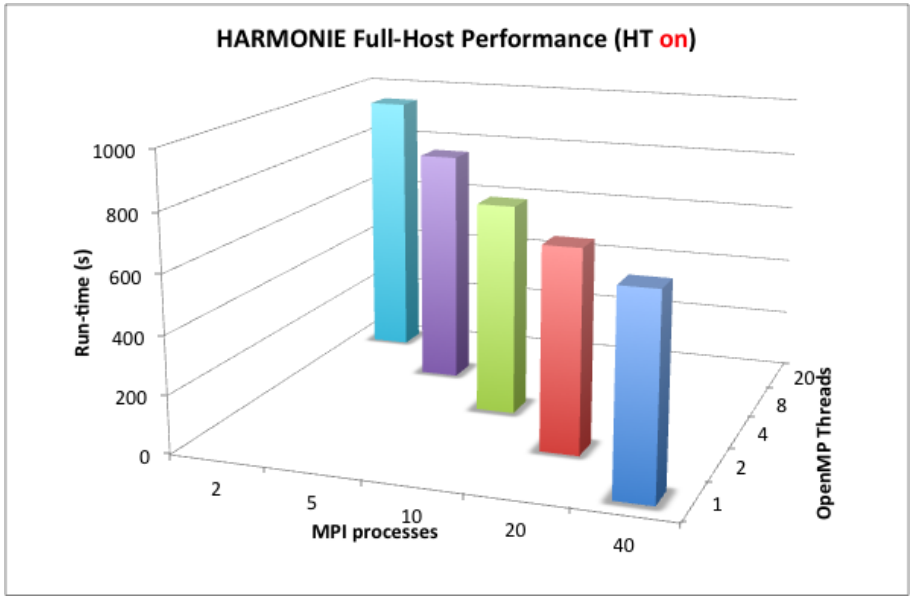
- **Fine-grained**: each loop is a separate OMP parallel region
- **Partial Coarse-grained**: Single high-level OpenMP parallel region
- **Full Coarse-grained**: Data fully decomposed to be thread-aware (as well as MPI-aware). Requires more, smaller MPI messages!

HARMONIE Parallel "Mix": OpenMP or MPI?

Xeon host node, without HT:



With HT:



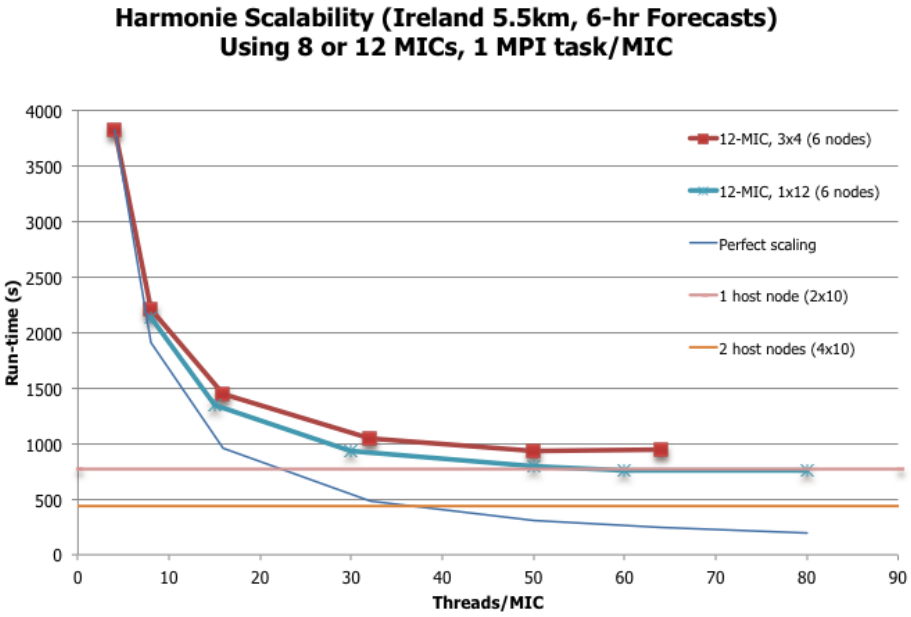
Conclusion:
For HARMONIE on Xeon nodes, MPI performs better than OpenMP.

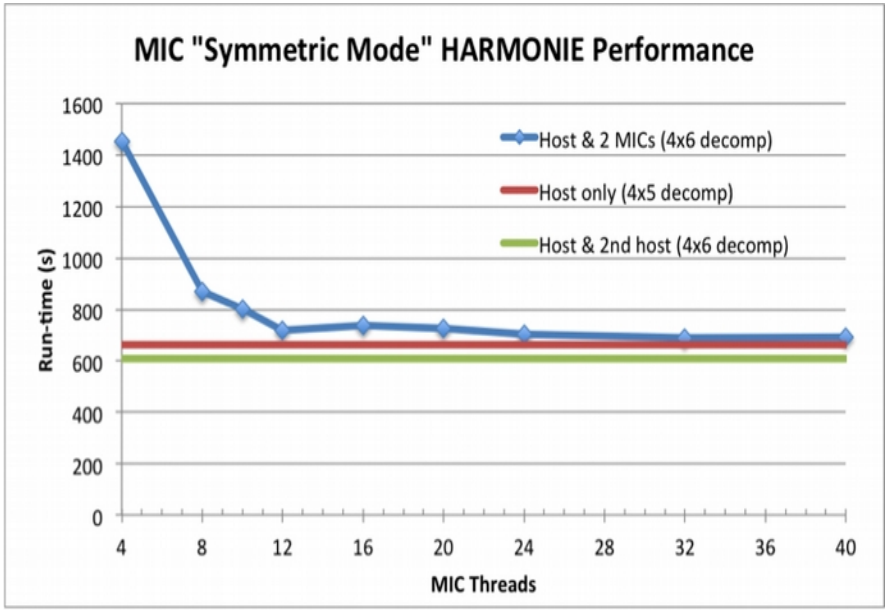
Alternative Conclusion:
OpenMP in HARMONIE is not yet optimized!

HARMONIE on Xeon Phi Coprocessors

- HARMONIE can run on Xeon Phi Coprocessors, in either:
  - "Native" mode (full job run on Phi)
  - "Symmetric" mode (some MPI tasks on Phis, some on hosts)
  - "Offload" mode (some code-sections or "kernels" are transferred to Phi to be run there)
- Performance is poor – partly because HARMONIE runs out of memory before running out of cores (or threads)!
  - Memory use increases almost in proportion to thread-count!
- *Cy40 changes should be able to avoid memory blow-up!*
  - Still need to be tested, esp. on Xeon Phi…

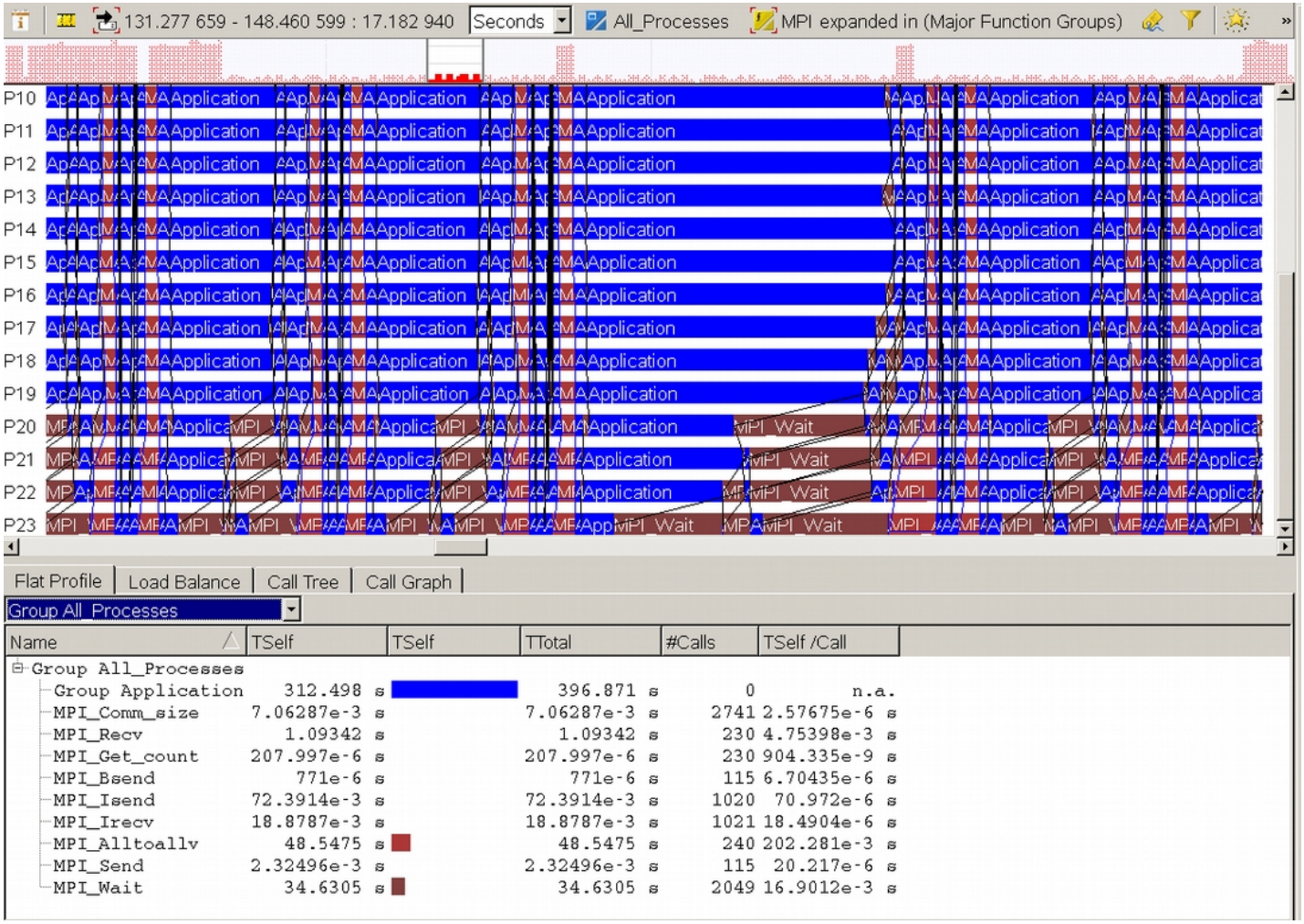
Harmonie Scalability on MIC (Native & Symmetric modes)





One node; 20-tasks on host,
2 tasks on each of 2 MICs

HARMONIE: Symmetric Mode load (im)balance



Approx. 5 Harmonie timesteps; 20 host & 4 MIC processes

Symmetric Mode Profiles (20 host + 4 MIC MPIs)

Host Profile (20 MPI x 2 threads)	
Routine	% run-time
LAITRI @thread	4.4
APL_AROME @thread	4.3
RRTM_RTRN1A* @thread	3.2
TRLTOM	3.1
TRLTOG	3.0
TRMTOL	2.9
EGPNORM_TRANS	2.9
CPG	2.8
SLCOMM2A	2.7
INITAPLPAR @thread	2.2
GATHFLNM<RECV	2.1

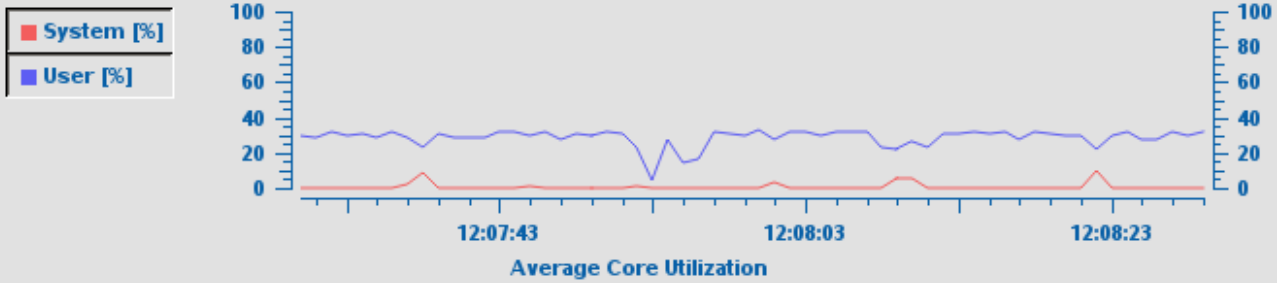
MIC Prof (2 MIC x 2 MPI x 32 thrd)	
Routine	% run-time
SLCOMM	26.0
TRLTOG	7.0
SLCOMM2A	5.9
TRGTOL	3.7
TRMTOL	3.3
CPG	2.4
RRTM_RTRN1A* @thread	2.1
TRMTOS	2.0
TRLTOM	1.9
LAITRI @thread	1.7
APL_AROME @thread	1.7

(SLCOMM dominance on MICs indicates load imbalance; MIC tasks waiting for host messages)

Intel® Xeon Phi™ Coprocessor Platform Status Panel

Cards | Advanced | Cards: 2 | Memory: 16 GB | Cores: 12

Utilization View (All Devices)

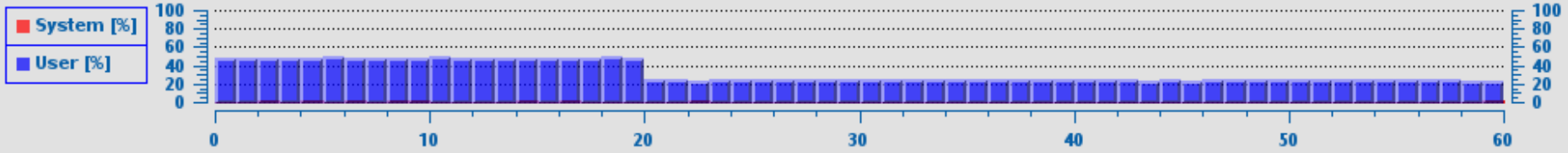


44
Average Core Temperature °C

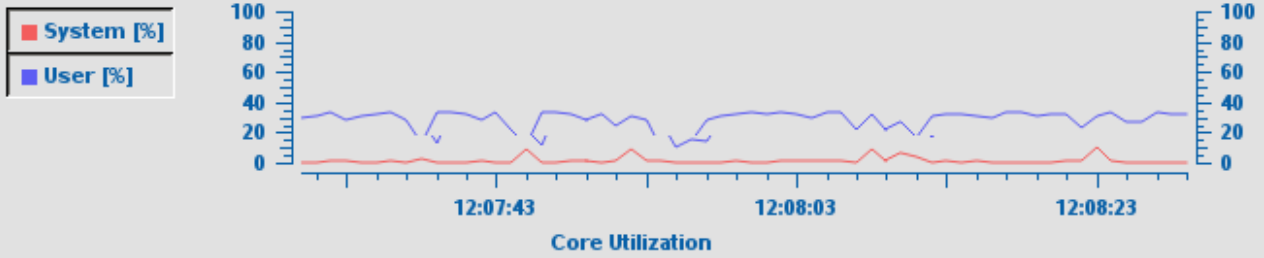
14.534 GB
Total Memory Usage

260 Watts
Total Power Usage

mic0: Core Histogram View



mic1: Utilization View



41
Processor Core Temperature °C

7212.2 MB
Memory Usage

132 Watts
Power Usage

For All Platforms…

- Harmonie has both MPI and OpenMP parallelism.
- OpenMP directives are at a very high level in source.
- Even so, memory usage is nearly proportional to thread-count – why?
- Turns out that main working-array sizes are simply increased in size to accommodate each new thread.
  - Okay for OMP_NUM_THREADS=2 or 4, perhaps
  - Definitely not okay for OMP_NUM_THREADS ≳ 10 (never mind 240!)
  - Reflects a "partial" implementation of "coarse-grained" multithreading.

High-level OpenMP Parallel Section (CPG)

"Working" arrays are declared (e.g., cpg.F90):

```
REAL*8 :: ARRAY(NPROMA,NLEV,KBLKS)
```

Where:

NPROMA = Sequential "block" size (for optimal cache use), ~30 for scalar processors.
NLEV = no. of vertical levels (~60 or 90)
KBLKS = 1 (MPI-only), or OMP_NUM_THREADS

(Total horizontal grid-points is **NGPTOT** (~100,000) – not used in array declarations)

```
!$OMP PARALLEL DO PRIVATE(J,L,…)
DO J = 1, NGPTOT, NPROMA
   !(calculate offsets, start & end pts. etc.)
   ...
   L = OML_MY_THREAD
   CALL CPG_GP(J, L, ARRAY(1,1,L),...)
   ...
ENDDO
```

Arrays in CPG_GP are then just 2-D: ARRAY(NPROMA,NLEV).

Final working arrays ultimately saved to large pointer-based state structure.

Highly parallel, but profligate with memory!

This is (Roughly…) Equivalent to:

```
REAL*8 :: ARRAY(NPROMA,NLEV) ! Smaller size – but OMP "private"
```

Where:

NPROMA = Sequential block size, as before.

NLEV = No. of vertical levels, as before

(Total horizontal grid-points is **NGPTOT** (~100,000) – not used in array declarations)

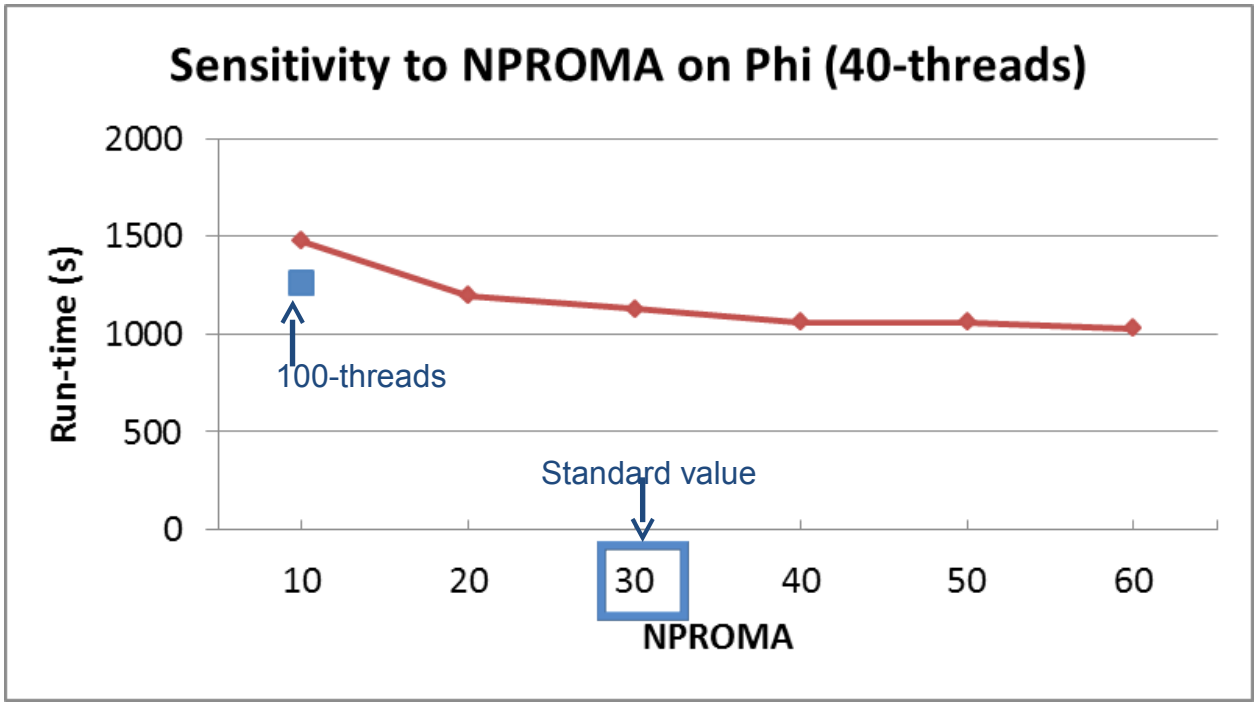
```
!$OMP PARALLEL DO PRIVATE(J,ARRAY,...)
DO J = 1, NGPTOT, NPROMA
   !(calculate offsets, start & end pts. etc.)
   ...
   CALL CPG_GP(J, ARRAY,...)
   ...
ENDDO
```

Using arrays as OpenMP "private" variables multiplies use of memory!

How about just reducing NPROMA?

Reducing NPROMA certainly allows use of more threads on Phi.

- However, performance not much better.
- For fixed thread-count, performance is better for larger NPROMA:



Can we re-factor to save memory?

"Working" arrays could be declared:

```
REAL*8 :: ARRAY(NLEV,NPROMA)   ! Switch dimensions
```

Where:

NPROMA = is ~10 x larger than before (to fill memory; e.g., ~4,000).
NLEV = no. of vertical levels as before

Parallelize over the (new, larger) NPROMA, as in:

```
THRED_BLK_SZ = NPROMA/OMP_NUM_THREADS
DO I = 1,NBLKS              ! (NBLKS ~ NGPTOT/NPROMA)
    !(calculate offsets, start & end pts. etc.)
  !$OMP PARALLEL DO PRIVATE(J,L,...)
  DO J = 1, NPROMA, THRED_BLK_SZ
    L = OML_MY_THREAD()
    CALL CPG_GP(I,J,L, THRED_BLK_SZ, ARRAY(1,L),...)
    ...
  ENDDO
ENDDO
```

Vertical depencies in CPG_GP, etc. are handled naturally (thread-local).

One extra transpose required at end (to save in (x,z) order again).

Worth further exploration!(?)

High-level OpenMP in Cycle-40

"Working" arrays are declared (e.g., cpg_drv.F90):

```
REAL*8 :: ARRAY(NPROMA,NFLEVG,NGPBLKS)
```

Where:

NPROMA = Sequential "block" size (for optimal cache use, ~30).
NFLEVG = no. of vertical levels (~60 or 90)
NGPBLKS = No. of "blocks" in NGPTOT; *independent of OMP_NUM_THREADS*

(Total horizontal grid-points is **NGPTOT** (~100,000) – not used in array declarations)

```
!$OMP PARALLEL DO PRIVATE(J,IBL,…)
DO J = 1, NGPTOT, NPROMA
   !(calculate offsets, start & end pts. etc.)
   ...
   IBL = (J-1)/NPROMA+1 ! Block index; not tied to any thread
   CALL CPG(J, IBL, ARRAY(1,1,IBL),...)
   ...
ENDDO
```

Arrays in CPG are then just 2-D: ARRAY(NPROMA,NFLEVG).

Each thread still works on on entire NPROMA-sized "block"; still highly parallel.

This decoupling of NGPBLKS from OMP_NUM_THREADS from might work!

Characteristics of Cycle-40 Design

- ✓ Approx. constant memory use as thread-count varies…
  - … though at a much higher level than in Cy38 (MPI-only).
  - No net improvement if NGPBLKS > OMP_NUM_THREADS.
- ✓ Any other changes required already made by Tomas Wilhelmsson!
- ✓ NPROMA can play exactly the same role as before (cache-blocking).

Needs to be tested, especially on Xeon Phi!