Hewlett Packard Enterprise

Preparing an application for Hybrid Supercomputing

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Senior Distinguished Technologist

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Agenda

- Introduction and a Little History
- Steps in moving an application to a GPU
- A simple example - himeno
- Optimizing himeno – with openmp on the node
- Optimizing himeno – with openmp offload on the GPUs (or Openacc). DEMO
- Dealing with Halo exchanges DEMO

Introduction

Supercomputing and I have been around for around 55 years

The architecture we have today was first introduced in the last 55 years

We should learn from the past to prepare for the future

High level parallelism between many nodes – 1995 Beowulf

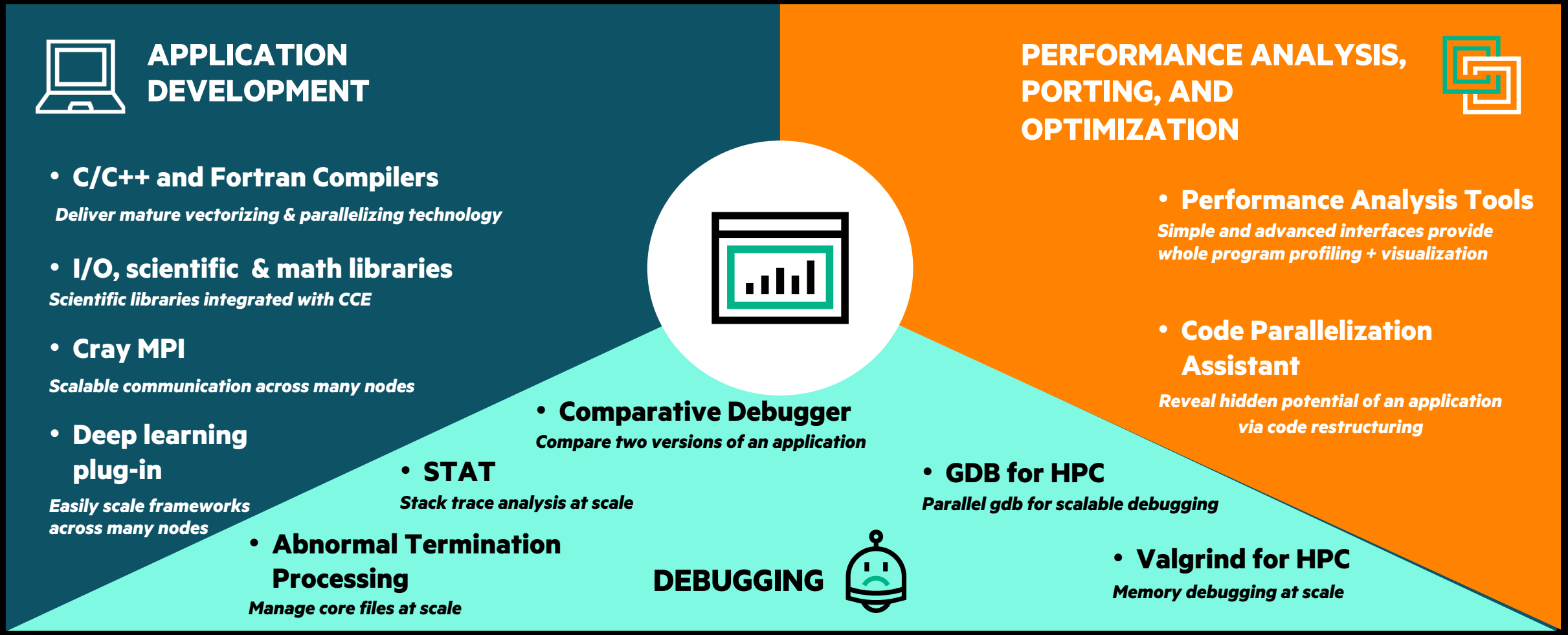
MIMD shared memory parallelism within the node – 1985 with Cray X-MP

Low level SIMD Parallelism - 1970 ILLIAC IV

Who is John Levesque?

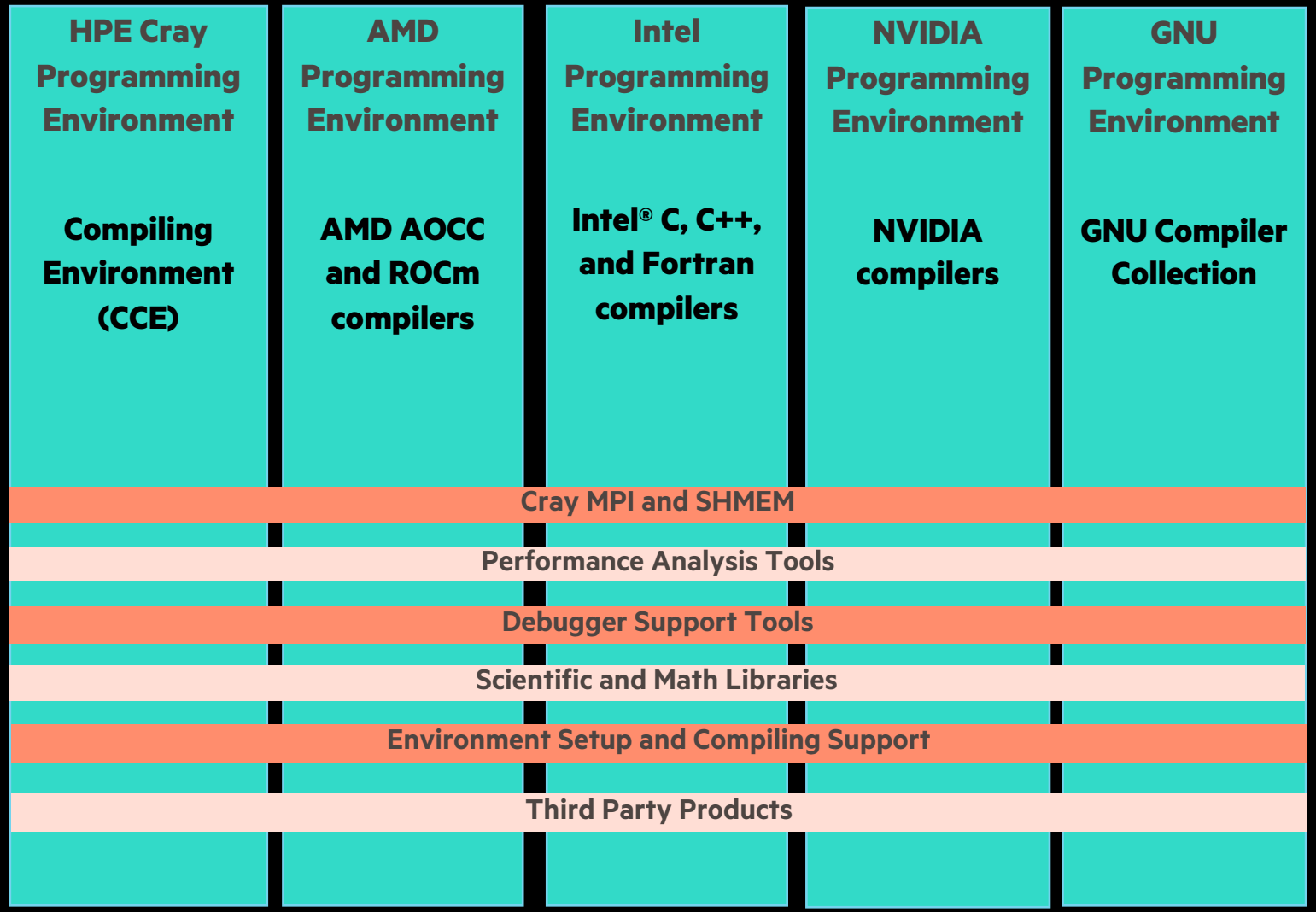
- 1964 – 1968
  - Delivered Meads Fine Bread, (Student at University of New Mexico 62-72)
- 3/1968 – 1970
  - Sandia Laboratories – Underground Physics Department (CDC3600)
- 1970 – 1972
  - Air Force Weapons Laboratory (CDC 6600)
- 1972 – 1978
  - R & D Associates - (CDC 7600, Illiac IV, Cray 1, Cyber 203-205)
- 1978 -1979
  - Massachusetts Computer Associates (Illiac IV, Cray 1) Parallizer
- 1979 – 1991
  - Pacific Sierra Research – (Intel Paragon, Ncube, Univac APS) - VAST
- 1991 – 1998
  - Applied Parallel Research – (MPPs of all sorts, CM5, NEC SX) – FORGE
- 1998 – 2001
  - IBM Research – Director Advanced Computing Technology Center
- 1/2001 – 9/2001
  - Times N Systems – Director of Software Development
- 9/2001 – 1/2021
  - Cray Inc – Director – Cray's Supercomputing Center of Excellence
- 1/2021 – 7/2024
  - HPE HPC/AI– Senior Distinguished Technologist – CTO Office

Complete and fully supported software development Suite



Providing the user with compiler choice

- Use modules to select compiling environment
  - Automatically uses our math, scientific, and communication libraries with chosen compiler
  - Can use debug and profiling tools with chosen compiler

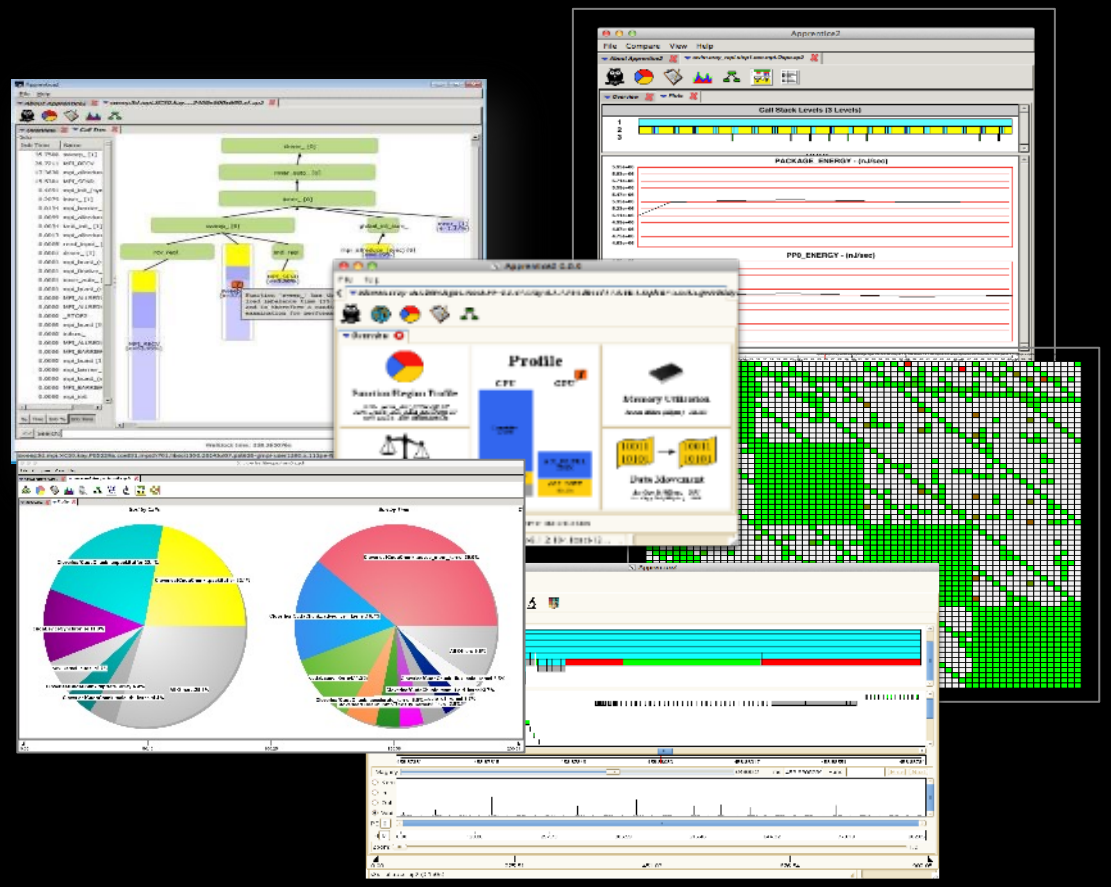


Performance Analysis Tools

Reduce time and effort associated with porting and tuning of applications on HPE systems

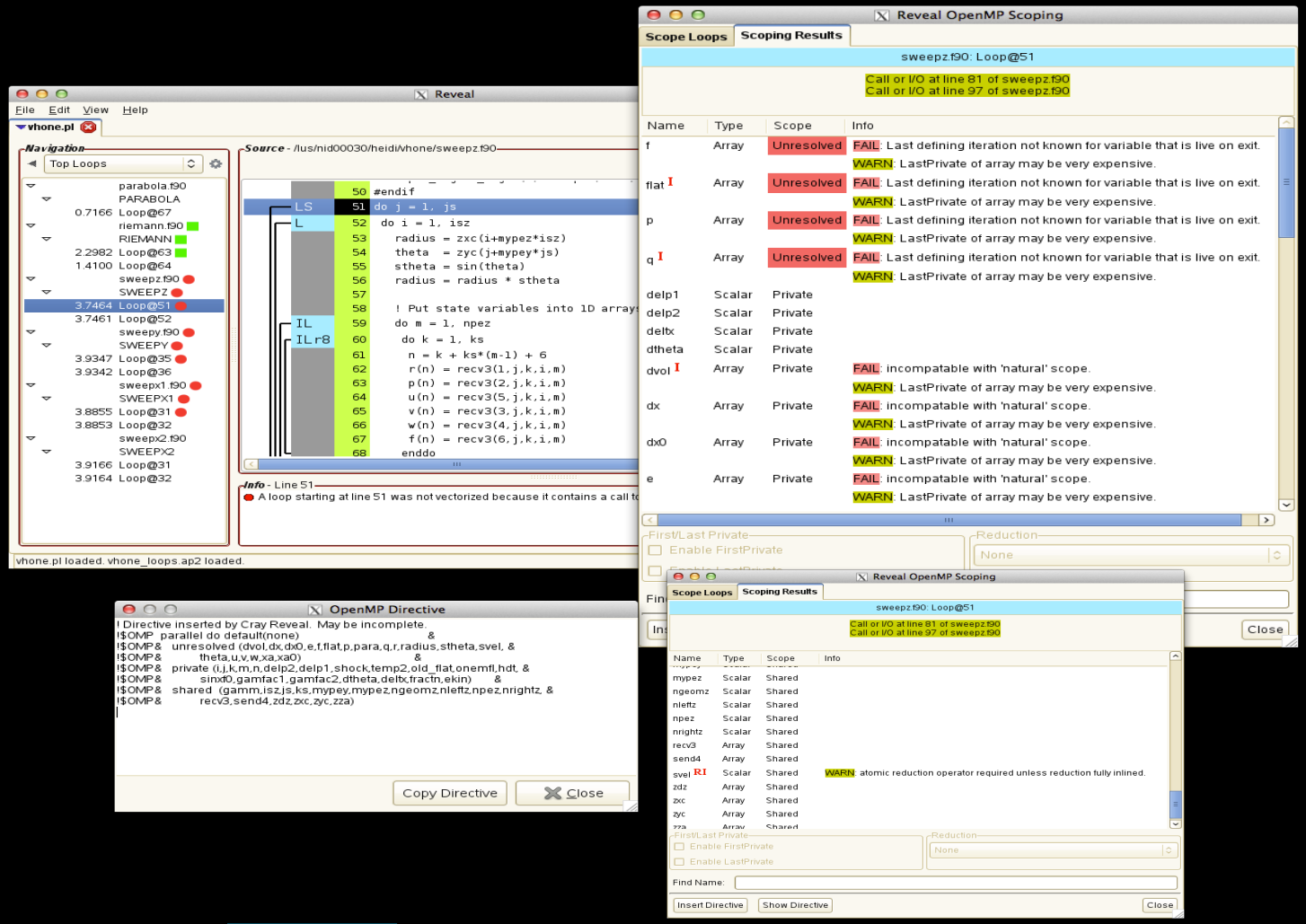
Highlights:

- Different tools to fit different developer needs—from quick visual analysis to variety of different experiments, integration with compilers and more…
- Target **scalability** issues in all areas of tool development—designed to improve performance on the largest of systems
- Provide **whole program performance analysis** across many nodes to identify critical performance bottlenecks in a program
- Help to uncover issues but also **suggestions to improve performance**
- Unique and valuable **load imbalance analysis**
- Target **ease of use** with simple and advanced user interfaces
- **Supports programs** written in Fortran, C or C++ with MPI, SHMEM, UPC, OpenMP or OpenACC, CUDA or HIP, and their combinations.



Our performance tools profiled production applications with over 256,000 ranks.

Code Parallelization Assistant



- Reduce effort associated with adding OpenMP to MPI programs
- Works in conjunction with our compiler and performance tools
- Easily navigate through source code to highlighted dependences or bottlenecks
- Identify work-intensive loops to parallelize, perform dependence analysis, scope variables and generate OpenMP directives
- Great first step when moving large, complex loops to GPUs

Directive-Based Programming Models

- Huge potential to provide cross-architecture portability (CPUs and GPUs)
- Standard specifications that all compiler vendors can implement
- Performance portability across vendors has been a recent challenge
- Has been critical for Fortran, especially for offloading
- OpenMP and OpenACC
  - Continued participation in language committees
  - Ongoing support for current and future specifications
  - Leverage common compiler and library codebase for OpenMP and OpenACC implementations
  - Significant opportunities for general performance improvements
  - Significant opportunities for improving construct-to-hardware mapping
    - Better cross-vendor consistency
    - Better use of descriptive features (e.g., “omp loop”)
    - Use of multidimensional grids, especially for “collapse” loops
- Specialized, low-level directive-based models may expand user base
  - Optimize performance for a limited set of OpenMP/OpenACC constructs and APIs
  - Provide a portable model similar to existing kernel languages (e.g., CUDA or HIP)

Using perftools-lite (or -loops or -hbm)

- module load perftools-lite or perftools-lite-loops or perftools-lite-hbm
  - Module perftools-base should already be loaded
- Build application
- Run application
- Statistics report comes out within standard out
  - Also generates a directory of profile data to be examined with different options

Lets start with a simple example

- cd himeno_hybrid
- module load perftools-lite
- ftn -rm himenoBMTxpr.f –ohimenox

```
[levesque@o185i082 himeno_hybrid]$ ftn -rm himenoBMTxpr.f  -ohimenox
WARNING: PerfTools is saving object files from a temporary directory into directory
'/lvol/levesque/.craypat/himenox/507153’
INFO: creating the PerfTools-instrumented executable 'himenox' (lite-samples) ...OK
```

- srun –n 2 ./himenox

Perftools-lite profile – Run on 1 nodes–2 MPI tasks/node

```
Table 1:  Profile by Function


  Samp% |    Samp | Imb.  |  Imb. | Group
        |         | Samp  | Samp% |  Function=[MAX10]
        |         |       |       |   PE=HIDE

 100.0% | 6,421.0 |   --  |    -- | Total
|-----------------------------------------------------
|  99.0% | 6,359.0 |   --  |    -- | USER
||----------------------------------------------------
||  98.8% | 6,341.0 | 51.0  |  1.6% | jacobi_
|====================================================
```

Exclusive time

Sampling is in

100th of a second

Imbalance

Only showing items that take up more than 1% of time – you can override with -T

Perftools-lite profile – Run on 1 nodes–2 MPI tasks/node

```
Table 1:  Profile by Function

  Samp% |    Samp | Imb. |   Imb. | Group
        |         | Samp |  Samp% |  Function
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 100.0% | 6,421.0 |   -- |     -- | Total
|-----------------------------------------------------
|  99.0% | 6,359.0 |   -- |     -- | USER
||----------------------------------------------------
||  98.8% | 6,341.0 | 51.0 |   1.6% | jacobi_
||   0.3% |    18.0 |  0.0 |   0.0% | initmt_
||====================================================
|   0.7% |    47.5 |   -- |     -- | MPI
||----------------------------------------------------
||   0.7% |    46.5 | 45.5 |  98.9% | MPI_WAITALL
||   0.0% |     0.5 |  0.5 | 100.0% | MPI_ISEND
||   0.0% |     0.5 |  0.5 | 100.0% | mpi_isend_
||====================================================
|   0.2% |    14.5 |  4.5 |  47.4% | ETC
||----------------------------------------------------
||   0.2% |    14.5 |  4.5 |  47.4% | __cray_memcpy_ROME
|=====================================================
```

pat_report -T himenox+507859-4242835s>profile_T

Exclusive time

Sampling is in

100th of a second

Imbalance

Perftools-lite profile – Run on 1 nodes–2 MPI tasks/node

```
Table 2:  Profile of maximum function times
```

pat_report -T himenox+507859-4242835s>profile_T

Samp%	Samp	Imb. Samp	Imb. Samp%	Function / PE
100.0%	6,392.0	51.0	1.6%	jacobi_
100.0%	6,392.0	--	--	pe.0
98.4%	6,290.0	--	--	pe.1
1.4%	92.0	45.5	98.9%	MPI_WAITALL
1.4%	92.0	--	--	pe.1
0.0%	1.0	--	--	pe.0
0.3%	19.0	4.5	47.4%	__cray_memcpy_ROME
0.3%	19.0	--	--	pe.1
0.2%	10.0	--	--	pe.0
0.3%	18.0	0.0	0.0%	initmt_
0.3%	18.0	--	--	pe.0
0.3%	18.0	--	--	pe.1

Exclusive time

Sampling is in

100th of a second

Imbalance

Perftools-lite profile – Run on 1 nodes–2 MPI tasks/node

Table 4: Program HW Performance Counter Data

pat_report -T himenox+507859-4242835s>profile_T

```
==========================================================================
  Total
--------------------------------------------------------------------------
  Thread Time                                     64.264144 secs
  CORE_TO_L2_CACHEABLE_REQUEST_ACCESS_STATUS:
    LS_RD_BLK_C                                5,977,290,738
  L2_PREFETCH_HIT_L2                           1,168,069,330
  L2_PREFETCH_HIT_L3                           2,141,277,288
  REQUESTS_TO_L2_GROUP1:L2_HW_PF               3,775,988,456
  REQUESTS_TO_L2_GROUP1:RD_BLK_X                 513,939,922
  Cache Lines PF from OffCore  0.041G/sec      2,607,919,126 lines
  Cache Lines PF from Memory   0.007G/sec        466,641,838 lines
  Cache Lines Requested from
    Memory                     0.017G/sec      1,069,532,376 lines
  Write Memory Traffic GBytes  0.063G/sec               4.06 GB
  Read Memory Traffic GBytes   1.530G/sec              98.32 GB
  Memory traffic GBytes        1.593G/sec             102.38 GB
  Memory Traffic / Nominal Peak                         0.8%
==========================================================================
```


Perftools-lite profile – Run on 1 nodes–2 MPI tasks/node

pat_report -T himenox+507859-4242835s>profile_T

```
Table 4:  Program HW Performance Counter Data

Notes for table 5:

  This table show the average time and number of bytes written to each
    output file, taking the average over the number of ranks that
    wrote to the file.  It also shows the number of write operations,
    and average rates.
  For further explanation, see the "General table notes" below, or
    use:  pat_report -v -O write_stats ...

Table 5:  File Output Stats by Filename

      Avg |      Avg |  Write Rate | Number |    Avg | Bytes/ | File Name
    Write |    Write | MiBytes/sec |     of | Writes |   Call |  PE=HIDE
 Time per |  MiBytes |             | Writer |    per |        |
   Writer |      per |             |  Ranks | Writer |        |
     Rank |   Writer |             |        |   Rank |        |
          |     Rank |             |        |        |        |
|-----------------------------------------------------------------
| 0.000018 | 0.000008 |    0.433920 |      2 |    1.0 |   8.00 | stderr
| 0.000003 | 0.000356 |  108.583797 |      2 |   11.0 |  33.91 | stdout
|=================================================================
```

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Perftools-lite profile – Run on 1 nodes–2 MPI tasks/node

```
Table 3:  Profile by Group, Function, and Line
```

pat_report -T himenox+507859-4242835s>profile_T

```
  Samp% |    Samp | Imb. |   Imb. | Group
        |         | Samp |  Samp% |  Function
        |         |      |        |   Source
        |         |      |        |    Line
        |         |      |        |     PE=HIDE


 100.0% | 6,421.0 |   -- |     -- | Total
|-------------------------------------------------------------------------
|  99.0% | 6,359.0 |   -- |     -- | USER
||------------------------------------------------------------------------
||  98.8% | 6,341.0 |   -- |     -- | jacobi_
3|        |         |      |        |  /lvol/levesque/himeno_hybrid/himenoBMTxpr.f
||||---------------------------------------------------------------------
4|||   1.6% |   105.5 |  1.5 |   2.8% | line.89
4|||   0.0% |     1.0 |  1.0 | 100.0% | line.213
4|||  85.9% | 5,518.5 |  6.5 |   0.2% | line.214
4|||   5.5% |   352.0 | 18.0 |   9.7% | line.224
4|||   1.6% |   101.0 |  8.0 |  14.7% | line.225
4|||   3.5% |   226.0 | 17.0 |  14.0% | line.226
4|||   0.6% |    37.0 |  1.0 |   5.3% | line.227
||||=====================================================================
```

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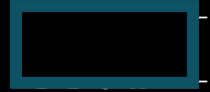
This is why we used –rm on ftn line (-h list=a)

```
200.                  C**************************************************************
201.                        subroutine jacobi(nn,gosa)
202.                  C**************************************************************
203.                        IMPLICIT REAL*4(a-h,o-z)
204.                  C
205.                        include 'mpif.h'
206.                        include 'param.h'
207.                  C
208.  + 1-----------<       DO loop=1,nn
209.    1                      gosa=0.0
210.    1                      wgosa=0.0
211.  + 1 2----------<         DO K=2,kmax-1
212.  + 1 2 3--------<           DO J=2,jmax-1
213.    1 2 3 Vr3----<             DO I=2,imax-1
214.    1 2 3 Vr3                    S0=a(I,J,K,1)*p(I+1,J,K)+a(I,J,K,2)*p(I,J+1,K)
215.    1 2 3 Vr3          1              +a(I,J,K,3)*p(I,J,K+1)
216.    1 2 3 Vr3          2              +b(I,J,K,1)*(p(I+1,J+1,K)-p(I+1,J-1,K)
217.    1 2 3 Vr3          3              -p(I-1,J+1,K)+p(I-1,J-1,K))
218.    1 2 3 Vr3          4              +b(I,J,K,2)*(p(I,J+1,K+1)-p(I,J-1,K+1)
219.    1 2 3 Vr3          5              -p(I,J+1,K-1)+p(I,J-1,K-1))
220.    1 2 3 Vr3          6              +b(I,J,K,3)*(p(I+1,J,K+1)-p(I-1,J,K+1)
221.    1 2 3 Vr3          7              -p(I+1,J,K-1)+p(I-1,J,K-1))
222.    1 2 3 Vr3          8              +c(I,J,K,1)*p(I-1,J,K)+c(I,J,K,2)*p(I,J-1,K)
223.    1 2 3 Vr3          9              +c(I,J,K,3)*p(I,J,K-1)+wrk1(I,J,K)
224.    1 2 3 Vr3                    SS=(S0*a(I,J,K,4)-p(I,J,K))*bnd(I,J,K)
225.    1 2 3 Vr3                    WGOSA=WGOSA+SS*SS
226.    1 2 3 Vr3                    wrk2(I,J,K)=p(I,J,K)+OMEGA *SS
227.    1 2 3 Vr3---->             enddo
228.    1 2 3-------->           enddo
229.    1 2---------->         enddo
230.    1              C
231.  + 1 2----------<         DO K=2,kmax-1
232.  + 1 2 3--------<           DO J=2,jmax-1
233.                  ---<         DO I=2,imax-1
234.                                 p(I,J,K)=wrk2(I,J,K)
235.                  --->         enddo
236.    1 2 3-------->           enddo
237.    1 2---------->         enddo
```



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Perftools-lite profile – Run on 1 nodes–2 MPI tasks/node

```
Table 3:  Profile by Group, Function, and Line
```

pat_report -T himenox+507859-4242835s>profile_T

```
  Samp% |    Samp | Imb. |   Imb. | Group
        |         | Samp |  Samp% |  Function
        |         |      |        |   Source
        |         |      |        |    Line
        |         |      |        |     PE=HIDE

 100.0% | 6,421.0 |   -- |     -- | Total
|-----------------------------------------------------------------------
|  99.0% | 6,359.0 |   -- |     -- | USER
||----------------------------------------------------------------------
||  98.8% | 6,341.0 |   -- |     -- | jacobi_
3|        |         |      |        |  /lvol/levesque/himeno_hybrid/himenoBMTxpr.f
||||---------------------------------------------------------------------
4|||   1.6% |   105.5 |  1.5 |   2.8% | line.89
4|||   0.0% |     1.0 |  1.0 | 100.0% | line.213
4|||  85.9% | 5,518.5 |  6.5 |   0.2% | line.214
4|||   5.5% |   352.0 | 18.0 |   9.7% | line.224
4|||   1.6% |   101.0 |  8.0 |  14.7% | line.225
4|||   3.5% |   226.0 | 17.0 |  14.0% | line.226
4|||   0.6% |    37.0 |  1.0 |   5.3% | line.227
||||=====================================================================
```

Lets Optimize this code

- Shared memory parallelism
- Put on the GPU
- To do these things we need to understand the loop limits

```
module  swap perftools-lite perftools-lite-loops
ftn -rm himenoBMTxpr.f -ohimenox
WARNING: PerfTools is saving object files from a temporary directory into directory
'/lvol/levesque/.craypat/himenox/508047’
INFO: creating the PerfTools-instrumented executable 'himenox' (lite-loops) ...OK
srun –n 2 ./himenox
```


pat_report -T -Oct himenox+508124-4242835t>profile_Tloops_ct

Perftools-lite-loops profile – Run on 1 nodes–2 MPI tasks/node

```
Table 1:  Calltree with Loop Inclusive Time
   Incl |   Incl | Loop Exec |  Loop | Calltree
  Time% |   Time |           | Trips |  PE=HIDE
        |        |           |   Avg |
 100.0% |  63.50 |        -- |    -- | Total
|-------------------------------------------------------------
| 100.0% |  63.50 |        -- |    -- | himenobmtxp_
||------------------------------------------------------------
|| 197.3% | 125.31 | 2,331,148 | 126.5 | jacobi_
|||-----------------------------------------------------------
3||  99.4% |  63.14 |         2 |  74.0 | jacobi_.LOOP.1.li.208
||||----------------------------------------------------------
4|||  98.6% |  62.61 |       148 | 125.0 | jacobi_.LOOP.2.li.211
4|||   0.3% |   0.21 |    18,500 | 125.0 | jacobi_.LOOP.6.li.232
|||||---------------------------------------------------------
5||||   0.2% |   0.10 | 2,312,500 | 126.5 | jacobi_.LOOP.7.li.233
|||===========================================================
||   0.6% |   0.35 |    16,256 | 128.5 | initmt_
|||-----------------------------------------------------------
3||   0.3% |   0.20 |         1 | 128.0 | initmt_.LOOP.1.li.154
||||----------------------------------------------------------
4|||   0.3% |   0.20 |       128 | 128.0 | initmt_.LOOP.2.li.155
|||||---------------------------------------------------------
5||||   0.3% |   0.19 |    16,384 | 128.0 | initmt_.LOOP.3.li.156
||||==========================================================
3||   0.2% |   0.16 |         1 | 127.0 | initmt_.LOOP.4.li.175
|||===========================================================
||   0.0% |   0.00 |         0 |    -- | _STOP3
||   0.0% |   0.00 |        -- |    -- | initcomm_
|||-----------------------------------------------------------
3||   0.0% |   0.00 |         0 |    -- | mpi_init_(sync)
3||   0.0% |   0.00 |         0 |    -- | MPI_INIT
|||===========================================================
||   0.0% |   0.00 |         0 |    -- | mpi_finalize_(sync)
||   0.0% |   0.00 |        -- |    -- | initmax_
|||-----------------------------------------------------------
3||   0.0% |   0.00 |         1 |   2.0 | initmax_.LOOP.1.li.352
3||   0.0% |   0.00 |         1 |   2.0 | initmax_.LOOP.2.li.359
|||===========================================================
```

This is why we used –rm on ftn line (-h list=a)

```
200.                  C**************************************************************
201.                        subroutine jacobi(nn,gosa)
202.                  C**************************************************************
203.                        IMPLICIT REAL*4(a-h,o-z)
204.                  C
205.                        include 'mpif.h'
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208.  + 1-----------<       DO loop=1,nn
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215.    1 2 3 Vr3          1              +a(I,J,K,3)*p(I,J,K+1)
216.    1 2 3 Vr3          2              +b(I,J,K,1)*(p(I+1,J+1,K)-p(I+1,J-1,K)
217.    1 2 3 Vr3          3              -p(I-1,J+1,K)+p(I-1,J-1,K))
218.    1 2 3 Vr3          4              +b(I,J,K,2)*(p(I,J+1,K+1)-p(I,J-1,K+1)
219.    1 2 3 Vr3          5              -p(I,J+1,K-1)+p(I,J-1,K-1))
220.    1 2 3 Vr3          6              +b(I,J,K,3)*(p(I+1,J,K+1)-p(I-1,J,K+1)
221.    1 2 3 Vr3          7              -p(I+1,J,K-1)+p(I-1,J,K-1))
222.    1 2 3 Vr3          8              +c(I,J,K,1)*p(I-1,J,K)+c(I,J,K,2)*p(I,J-1,K)
223.    1 2 3 Vr3          9              +c(I,J,K,3)*p(I,J,K-1)+wrk1(I,J,K)
224.    1 2 3 Vr3                    SS=(S0*a(I,J,K,4)-p(I,J,K))*bnd(I,J,K)
225.    1 2 3 Vr3                    WGOSA=WGOSA+SS*SS
226.    1 2 3 Vr3                    wrk2(I,J,K)=p(I,J,K)+OMEGA *SS
227.    1 2 3 Vr3---->             enddo
228.    1 2 3-------->           enddo
229.    1 2---------->         enddo
230.    1              C
231.  + 1 2----------<         DO K=2,kmax-1
232.  + 1 2 3--------<           DO J=2,jmax-1
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234.                                 p(I,J,K)=wrk2(I,J,K)
235.                  --->         enddo
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237.    1 2---------->         enddo
```

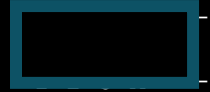

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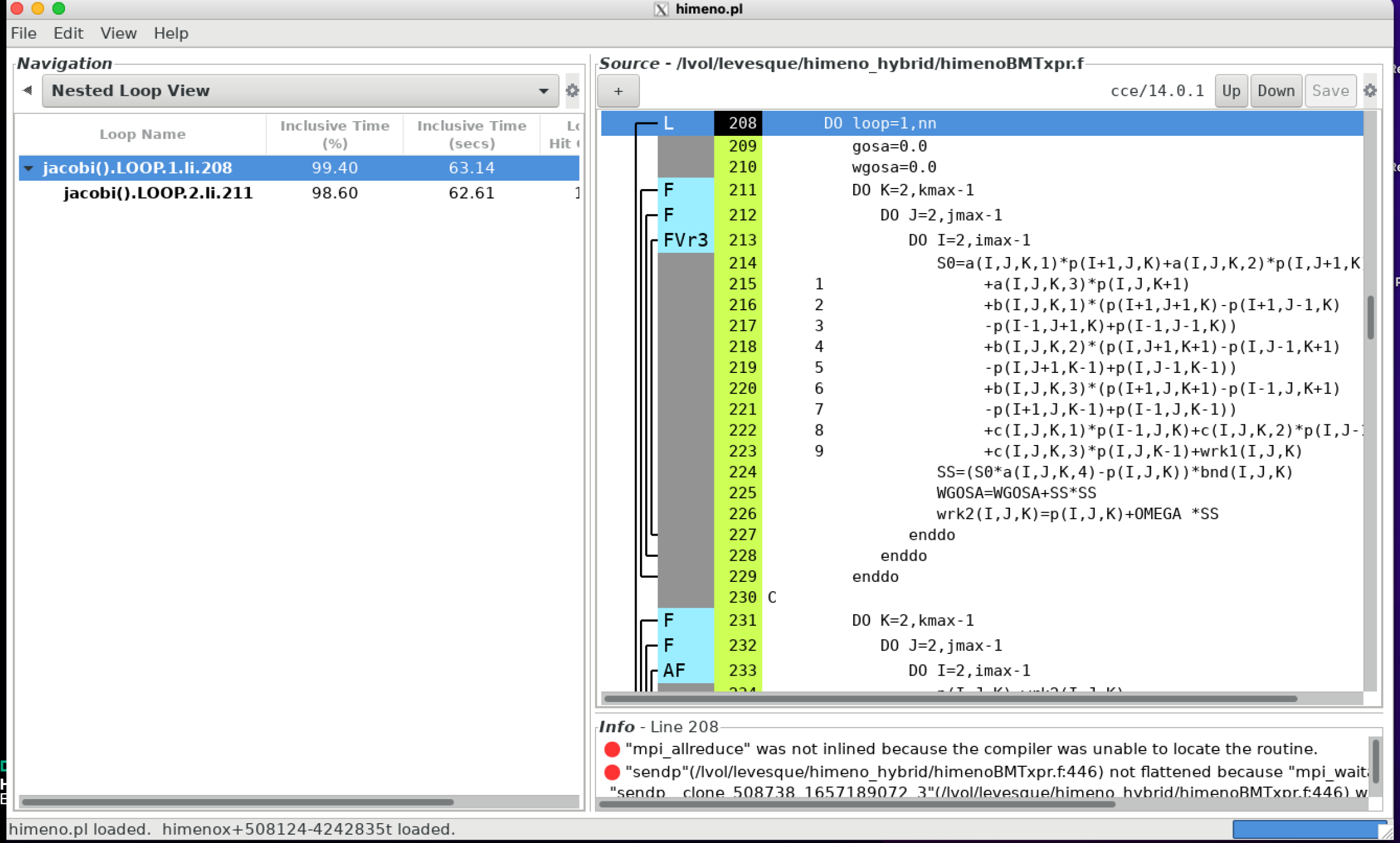
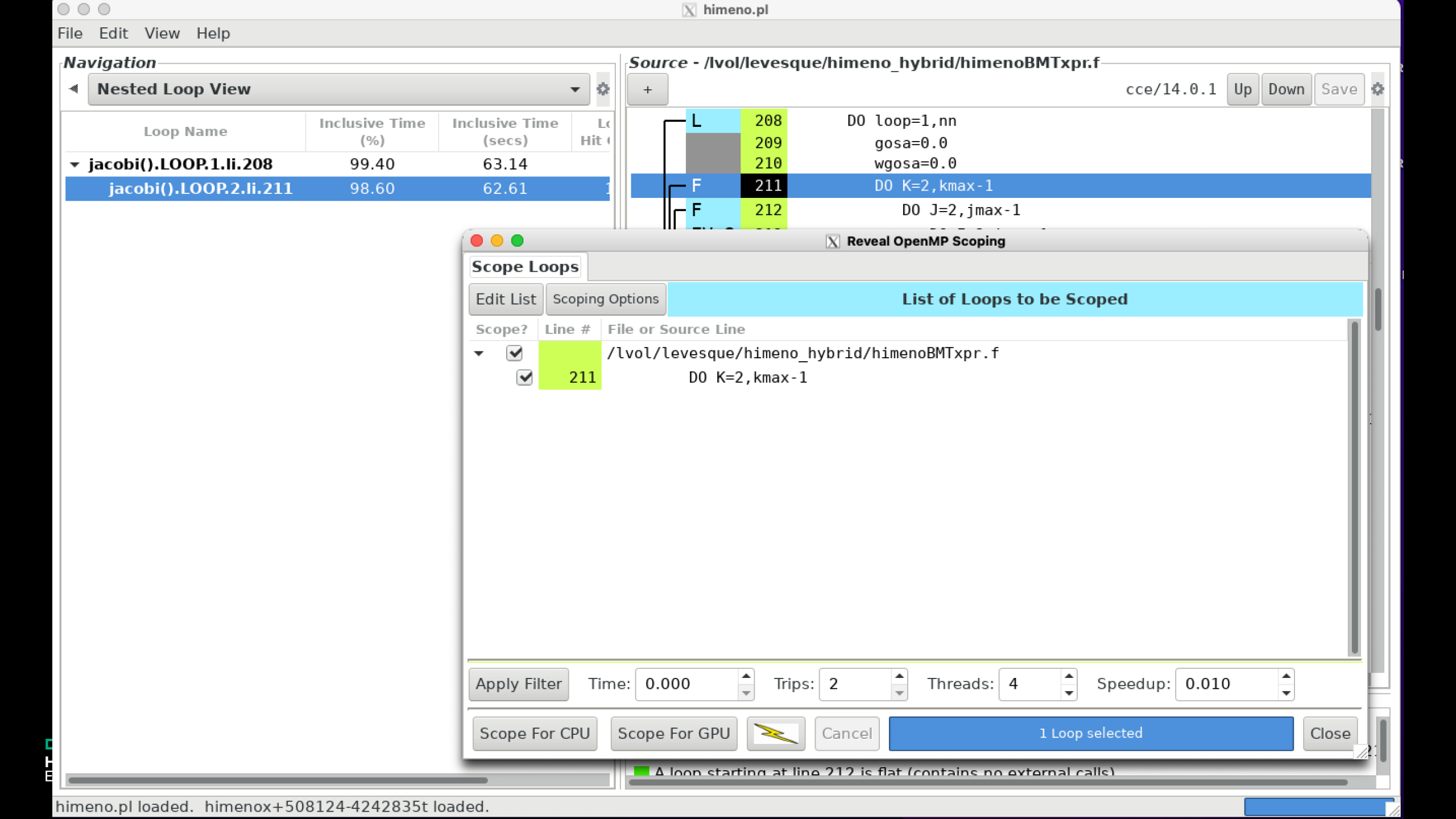
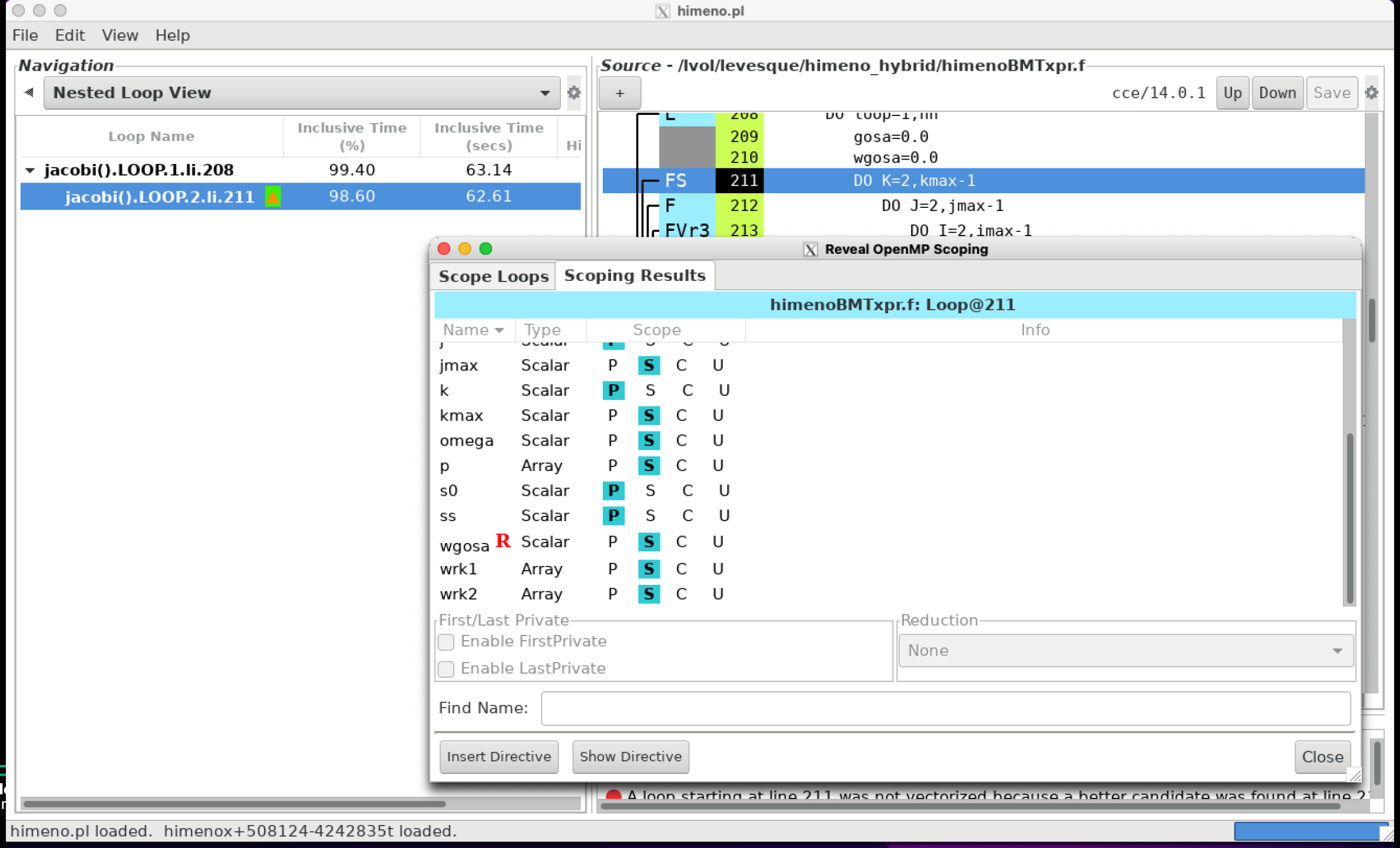
Lets Optimize this code

- Shared memory parallelism
- We have a tool called reveal to help parallelize code for host and CPU
- We need to build a program library to use reveal

```
module unload perftools-lite-loops
ftn –hpl=himeno.pl himenoBMTxpr.f
reveal himeno.pl himenox+508124-4242835t
```



himeno.pl
File Edit View Help
Navigation
Nested Loop View
Loop Name
Inclusive Time (%)
Inclusive Time (secs)
jacobi().LOOP.1.li.208 99.40 63.14
jacobi().LOOP.2.li.211 98.60 62.61
Source - /lvol/levesque/himeno_hybrid/himenoBMTxpr.f
cce/14.0.1 Up Down Save
L 208 DO loop=1,nn
209 gosa=0.0
210 wgosa=0.0
F 211 DO K=2,kmax-1
F 212 DO J=2,jmax-1
FVr3 213 DO I=2,imax-1
214 S0=a(I,J,K,1)*p(I+1,J,K)+a(I,J,K,2)*p(I,J+1,K
215 1 +a(I,J,K,3)*p(I,J,K+1)
216 2 +b(I,J,K,1)*(p(I+1,J+1,K)-p(I+1,J-1,K)
217 3 -p(I-1,J+1,K)+p(I-1,J-1,K))
218 4 +b(I,J,K,2)*(p(I,J+1,K+1)-p(I,J-1,K+1)
219 5 -p(I,J+1,K-1)+p(I,J-1,K-1))
220 6 +b(I,J,K,3)*(p(I+1,J,K+1)-p(I-1,J,K+1)
221 7 -p(I+1,J,K-1)+p(I-1,J,K-1))
222 8 +c(I,J,K,1)*p(I-1,J,K)+c(I,J,K,2)*p(I,J-
223 9 +c(I,J,K,3)*p(I,J,K-1)+wrk1(I,J,K)
224 SS=(S0*a(I,J,K,4)-p(I,J,K))*bnd(I,J,K)
225 WGOSA=WGOSA+SS*SS
226 wrk2(I,J,K)=p(I,J,K)+OMEGA *SS
227 enddo
228 enddo
229 enddo
230 C
F 231 DO K=2,kmax-1
F 232 DO J=2,jmax-1
AF 233 DO I=2,imax-1
Info - Line 208
"mpi_allreduce" was not inlined because the compiler was unable to locate the routine.
"sendp"(/lvol/levesque/himeno_hybrid/himenoBMTxpr.f:446) not flattened because "mpi_wait
himeno.pl loaded. himenox+508124-4242835t loaded.


himeno.pl
File Edit View Help
Navigation
Nested Loop View
Loop Name
Inclusive Time (%)
Inclusive Time (secs)
jacobi().LOOP.1.li.208
99.40
63.14
jacobi().LOOP.2.li.211
98.60
62.61
Source - /lvol/levesque/himeno_hybrid/himenoBMTxpr.f
cce/14.0.1
Up
Down
Save
L 208 DO loop=1,nn
209 gosa=0.0
210 wgosa=0.0
F 211 DO K=2,kmax-1
F 212 DO J=2,jmax-1
Reveal OpenMP Scoping
Scope Loops
Edit List
Scoping Options
List of Loops to be Scoped
Scope?
Line #
File or Source Line
/lvol/levesque/himeno_hybrid/himenoBMTxpr.f
211 DO K=2,kmax-1
Apply Filter
Time: 0.000
Trips: 2
Threads: 4
Speedup: 0.010
Scope For CPU
Scope For GPU
Cancel
1 Loop selected
Close
A loop starting at line 212 is flat (contains no external calls)
himeno.pl loaded. himenox+508124-4242835t loaded.


himeno.pl
File Edit View Help
Navigation
Nested Loop View
Loop Name
Inclusive Time (%)
Inclusive Time (secs)
jacobi().LOOP.1.li.208 99.40 63.14
jacobi().LOOP.2.li.211 98.60 62.61
Source - /lvol/levesque/himeno_hybrid/himenoBMTxpr.f
cce/14.0.1 Up Down Save
209 gosa=0.0
210 wgosa=0.0
FS 211 DO K=2,kmax-1
F 212 DO J=2,jmax-1
FVr3 213 DO I=2,imax-1
Reveal OpenMP Scoping
Scope Loops
Scoping Results
himenoBMTxpr.f: Loop@211
Name Type Scope Info
jmax Scalar P S C U
k Scalar P S C U
kmax Scalar P S C U
omega Scalar P S C U
p Array P S C U
s0 Scalar P S C U
ss Scalar P S C U
wgosa R Scalar P S C U
wrk1 Array P S C U
wrk2 Array P S C U
First/Last Private
Enable FirstPrivate
Enable LastPrivate
Reduction
None
Find Name:
Insert Directive
Show Directive
Close
himeno.pl loaded. himenox+508124-4242835t loaded.

himeno.pl

File Edit View Help

Navigation

Nested Loop View

Loop Name	Inclusive Time (%)	Inclusive Time (secs)	Hi
jacobi().LOOP.1.li.208	99.40	63.14	
jacobi().LOOP.2.li.211	98.60	62.61	

Source - /lvol/levesque/himeno_hybrid/himenoBMTxpr.f

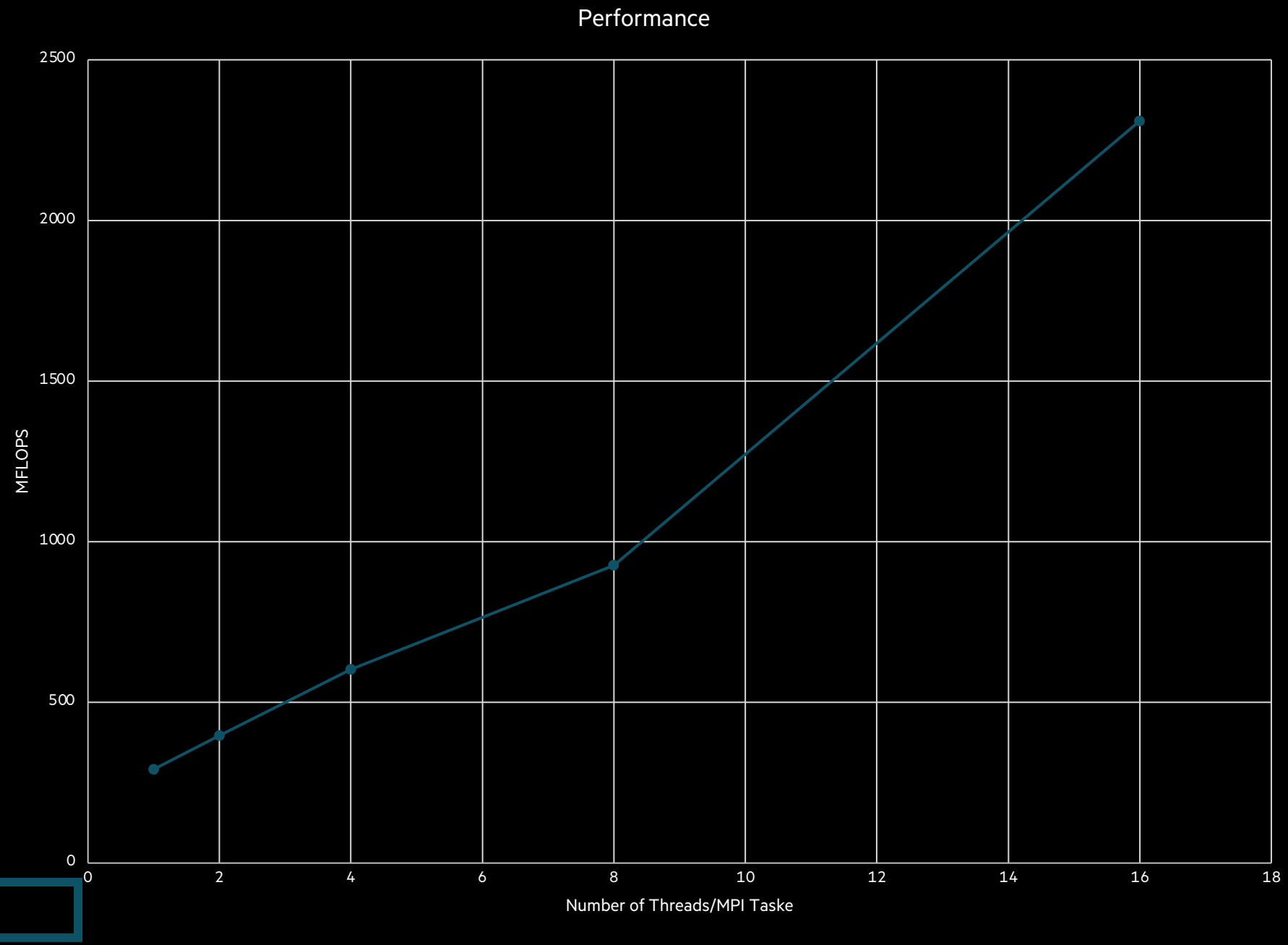
\+ cce/14.0.1 Up Down Save

```
205         include 'mpif.h'
206         include 'param.h'
207 C
L   208         DO loop=1,nn
209           gosa=0.0
210           wgosa=0.0
!  Directive inserted by Cray Reveal.  May be incomplete.
!$OMP  parallel do default(none)
!$OMP& shared(a, b, bnd, c, imax, jmax, kmax, omega, p, wgosa, w
!$OMP&  wrk2)
!$OMP& private(i, j, k, s0, ss)
!$OMP& reduction(+: wgosa)
FS  211           DO K=2,kmax-1
F   212             DO J=2,jmax-1
FVr3 213              DO I=2,imax-1
214                 S0=a(I,J,K,1)*p(I+1,J,K)+a(I,J,K,2)*p(I,J+1,K
215       1              +a(I,J,K,3)*p(I,J,K+1)
216       2              +b(I,J,K,1)*(p(I+1,J+1,K)-p(I+1,J-1,K)
217       3              -p(I-1,J+1,K)+p(I-1,J-1,K))
218       4              +b(I,J,K,2)*(p(I,J+1,K+1)-p(I,J-1,K+1)
219       5              -p(I,J+1,K-1)+p(I,J-1,K-1))
220       6              +b(I,J,K,3)*(p(I+1,J,K+1)-p(I-1,J,K+1)
221       7              -p(I+1,J,K-1)+p(I-1,J,K-1))
222       8              +c(I,J,K,1)*p(I-1,J,K)+c(I,J,K,2)*p(I,J-1
223       9              +c(I,J,K,3)*p(I,J,K-1)+wrk1(I,J,K)
224                 SS=(S0*a(I,J,K,4)-p(I,J,K))*bnd(I,J,K)
225                 WGOSA=WGOSA+SS*SS
226                 wrk2(I,J,K)=p(I,J,K)+OMEGA *SS
```

Info - Line 208

- "mpi_allreduce" was not inlined because the compiler was unable to locate the routine.
- "sendp"(/lvol/levesque/himeno_hybrid/himenoBMTxpr.f:446) not flattened because "mpi_wait
  "sendp__clone_508738_1657189072_3"(/lvol/levesque/himeno_hybrid/himenoBMTxpr.f:446) w

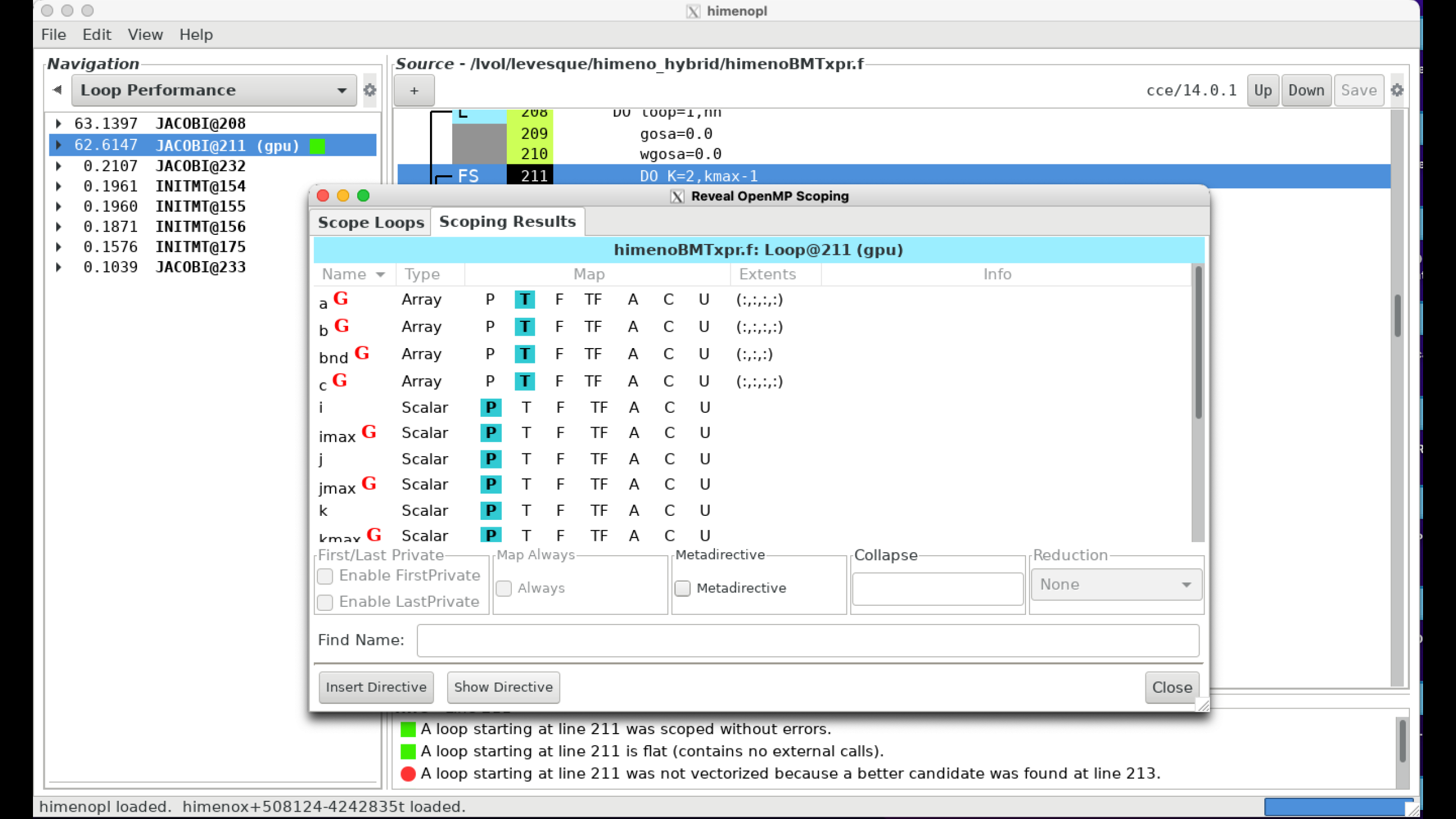
himeno.pl loaded. himenox+508124-4242835t loaded.

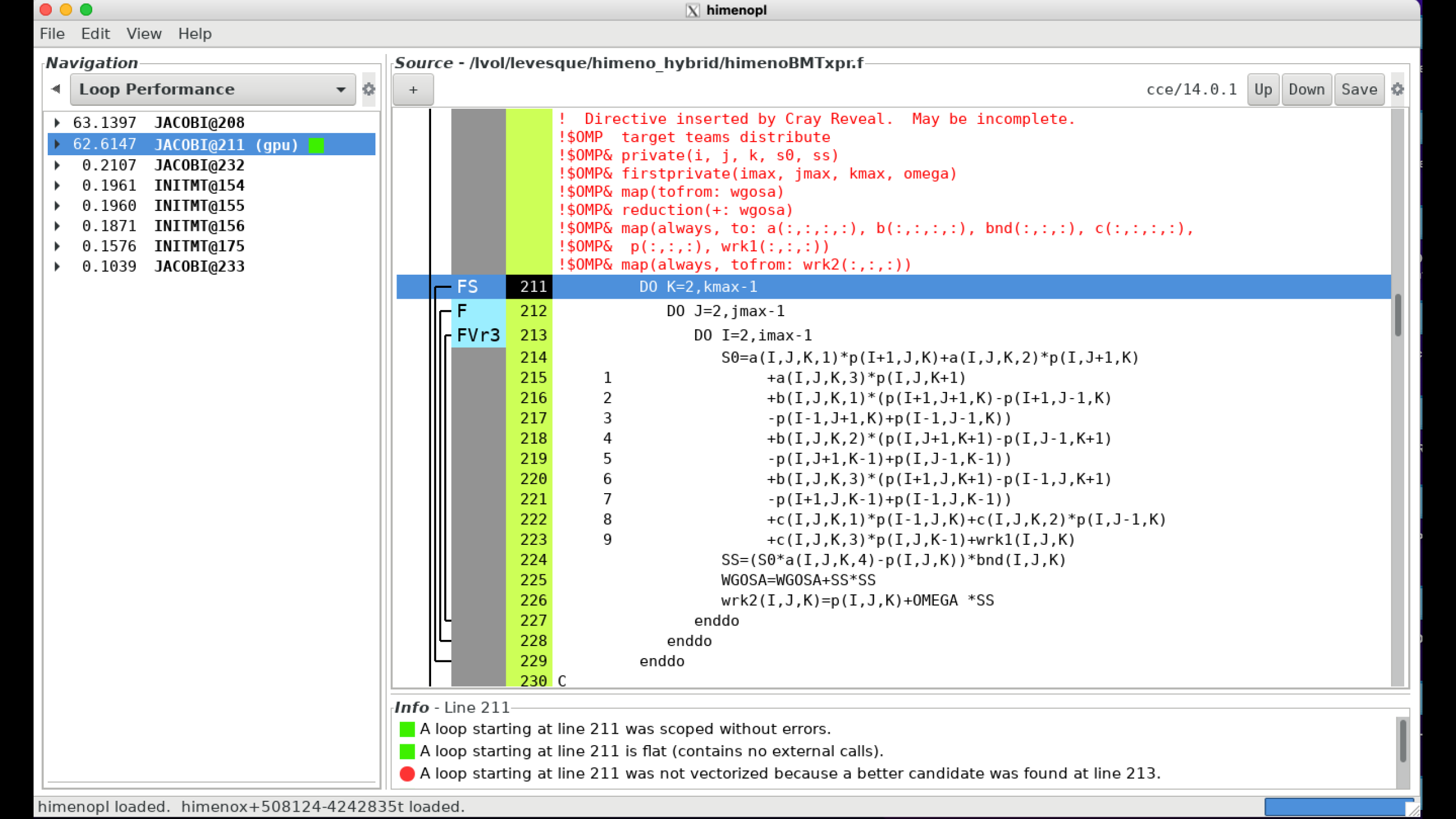


Hewlett Packard
Enterprise

Now lets put it on the GPU

- Go back to Reveal and generate GPU code

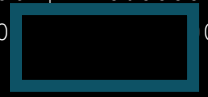

himenopl
File Edit View Help
Navigation
Loop Performance
63.1397 JACOBI@208
62.6147 JACOBI@211 (gpu)
0.2107 JACOBI@232
0.1961 INITMT@154
0.1960 INITMT@155
0.1871 INITMT@156
0.1576 INITMT@175
0.1039 JACOBI@233
Source - /lvol/levesque/himeno_hybrid/himenoBMTxpr.f
cce/14.0.1
Up
Down
Save
209 gosa=0.0
210 wgosa=0.0
FS 211 DO K=2,kmax-1
Reveal OpenMP Scoping
Scope Loops
Scoping Results
himenoBMTxpr.f: Loop@211 (gpu)
Name Type Map Extents Info
a G Array P T F TF A C U (:,:,:,:)
b G Array P T F TF A C U (:,:,:,:)
bnd G Array P T F TF A C U (:,:,:)
c G Array P T F TF A C U (:,:,:,:)
i Scalar P T F TF A C U
imax G Scalar P T F TF A C U
j Scalar P T F TF A C U
jmax G Scalar P T F TF A C U
k Scalar P T F TF A C U
kmax G Scalar P T F TF A C U
First/Last Private
Enable FirstPrivate
Enable LastPrivate
Map Always
Always
Metadirective
Metadirective
Collapse
Reduction
None
Find Name:
Insert Directive
Show Directive
Close
A loop starting at line 211 was scoped without errors.
A loop starting at line 211 is flat (contains no external calls).
A loop starting at line 211 was not vectorized because a better candidate was found at line 213.
himenopl loaded. himenox+508124-4242835t loaded.


himenopl
File Edit View Help
Navigation
Loop Performance
63.1397 JACOBI@208
62.6147 JACOBI@211 (gpu)
0.2107 JACOBI@232
0.1961 INITMT@154
0.1960 INITMT@155
0.1871 INITMT@156
0.1576 INITMT@175
0.1039 JACOBI@233
Source - /lvol/levesque/himeno_hybrid/himenoBMTxpr.f
+
cce/14.0.1
Up
Down
Save
! Directive inserted by Cray Reveal. May be incomplete.
!$OMP target teams distribute
!$OMP& private(i, j, k, s0, ss)
!$OMP& firstprivate(imax, jmax, kmax, omega)
!$OMP& map(tofrom: wgosa)
!$OMP& reduction(+: wgosa)
!$OMP& map(always, to: a(:,:,:,:), b(:,:,:,:), bnd(:,:,:), c(:,:,:,:),
!$OMP& p(:,:,:), wrk1(:,:,:))
!$OMP& map(always, tofrom: wrk2(:,:,:))
FS 211 DO K=2,kmax-1
F 212 DO J=2,jmax-1
FVr3 213 DO I=2,imax-1
214 S0=a(I,J,K,1)*p(I+1,J,K)+a(I,J,K,2)*p(I,J+1,K)
215 1 +a(I,J,K,3)*p(I,J,K+1)
216 2 +b(I,J,K,1)*(p(I+1,J+1,K)-p(I+1,J-1,K)
217 3 -p(I-1,J+1,K)+p(I-1,J-1,K))
218 4 +b(I,J,K,2)*(p(I,J+1,K+1)-p(I,J-1,K+1)
219 5 -p(I,J+1,K-1)+p(I,J-1,K-1))
220 6 +b(I,J,K,3)*(p(I+1,J,K+1)-p(I-1,J,K+1)
221 7 -p(I+1,J,K-1)+p(I-1,J,K-1))
222 8 +c(I,J,K,1)*p(I-1,J,K)+c(I,J,K,2)*p(I,J-1,K)
223 9 +c(I,J,K,3)*p(I,J,K-1)+wrk1(I,J,K)
224 SS=(S0*a(I,J,K,4)-p(I,J,K))*bnd(I,J,K)
225 WGOSA=WGOSA+SS*SS
226 wrk2(I,J,K)=p(I,J,K)+OMEGA *SS
227 enddo
228 enddo
229 enddo
230 C
Info - Line 211
A loop starting at line 211 was scoped without errors.
A loop starting at line 211 is flat (contains no external calls).
A loop starting at line 211 was not vectorized because a better candidate was found at line 213.
himenopl loaded. himenox+508124-4242835t loaded.

Commands for using perftools

- module swap perftools-lite-loops perftools
- ftn –hlist=a –homp himenoBMTxpr.f –o himenox
- pat_build –u –g mpi himenox
- srun –n 2 /himenox+pat
- pat_report –T <directory generated by execution>

```
Table 1:  Profile by Function Group and Function
  Time% |       Time | Imb. Time |   Imb. |     Calls | Group
        |            |           |  Time% |           |  Function
        |            |           |        |           |   PE=HIDE
        |            |           |        |           |    Thread=HIDE
 100.0% | 517.005427 |        -- |     -- | 170,510.0 | Total
|-------------------------------------------------------------------------
|  93.2% | 482.005140 |        -- |     -- |  40,012.0 | OACC
||------------------------------------------------------------------------
||  86.8% | 448.955431 | 20.973100 |   6.0% |  10,000.0 | jacobi_.ACC_COPY@li.213
||   5.5% |  28.517275 |  2.813567 |  12.0% |  10,000.0 | jacobi_.ACC_COPY@li.239
||   0.5% |   2.609518 |  0.576732 |  24.1% |  10,000.0 | jacobi_.ACC_SYNC_WAIT@li.239
||   0.2% |   1.233697 |  0.009083 |   1.0% |       6.0 | jacobi_.ACC_COPY@li.89
||   0.1% |   0.687733 |  0.134373 |  21.8% |  10,000.0 | jacobi_.ACC_ASYNC_KERNEL@li.213
||   0.0% |   0.000823 |  0.000119 |  16.8% |       3.0 | jacobi_.ACC_ASYNC_KERNEL@li.89
||   0.0% |   0.000663 |  0.000142 |  23.4% |       3.0 | jacobi_.ACC_SYNC_WAIT@li.89
||========================================================================
|   3.9% |  20.382070 |        -- |     -- | 110,053.0 | MPI
||------------------------------------------------------------------------
||   3.3% |  17.007617 | 13.779150 |  59.7% |  20,006.0 | MPI_WAITALL
||   0.5% |   2.339848 |  1.328698 |  48.3% |  40,012.0 | MPI_ISEND
||   0.2% |   0.984848 |  0.743195 |  57.3% |  40,012.0 | MPI_IRECV
||   0.0% |   0.049582 |  0.002511 |   6.4% |  10,004.0 | MPI_ALLREDUCE
||   0.0% |   0.000066 |  0.000003 |   5.3% |       1.0 | MPI_CART_CREATE
||   0.0% |   0.000032 |  0.000005 |  17.7% |       1.0 | MPI_REDUCE
||   0.0% |   0.000027 |  0.000004 |  16.0% |       2.0 | MPI_BARRIER
||   0.0% |   0.000021 |  0.000002 |  10.9% |       4.0 | MPI_WTIME
||   0.0% |   0.000008 |  0.000006 |  52.7% |       2.0 | MPI_TYPE_COMMIT
||   0.0% |   0.000008 |  0.000001 |  20.2% |       2.0 | MPI_TYPE_VECTOR
||   0.0% |   0.000005 |  0.000000 |   3.9% |       1.0 | MPI_CART_GET
||   0.0%              03 |  0.000000 |   0.7% |       2.0 | MPI_CART_SHIFT
```



```
205.                    C
206.                          include 'mpif.h'
207.                          include 'param.h'
208.                    C
209.  + 1-------------<       DO loop=1,nn
210.    1                        gosa=0.0
211.    1                        wgosa=0.0
212.    1               !  Directive inserted by Cray Reveal.  May be incomplete.
213.  + 1 MG----------< !$OMP  target teams distribute
214.    1 MG            !$OMP& private(i, j, k, s0, ss)
215.    1 MG            !$OMP& firstprivate(imax, jmax, kmax, omega)
216.    1 MG            !$OMP& map(tofrom: wgosa)
217.    1 MG            !$OMP& reduction(+: wgosa)
218.    1 MG            !$OMP& map(always, to: a(:,:,:,:), b(:,:,:,:), bnd(:,:,:), c(:,:,:,:),
219.    1 MG            !$OMP&  p(:,:,:), wrk1(:,:,:))
220.    1 MG            !$OMP& map(always, tofrom: wrk2(:,:,:))
221.    1 MG g--------<          DO K=2,kmax-1
222.  + 1 MG g 4------<             DO J=2,jmax-1
223.    1 MG g 4 gr3--<                DO I=2,imax-1
224.    1 MG g 4 gr3                      S0=a(I,J,K,1)*p(I+1,J,K)+a(I,J,K,2)*p(I,J+1,K)
225.    1 MG g 4 gr3         1                 +a(I,J,K,3)*p(I,J,K+1)
226.    1 MG g 4 gr3         2                 +b(I,J,K,1)*(p(I+1,J+1,K)-p(I+1,J-1,K)
227.    1 MG g 4 gr3         3                 -p(I-1,J+1,K)+p(I-1,J-1,K))
228.    1 MG g 4 gr3         4                 +b(I,J,K,2)*(p(I,J+1,K+1)-p(I,J-1,K+1)
229.    1 MG g 4 gr3         5                 -p(I,J+1,K-1)+p(I,J-1,K-1))
230.    1 MG g 4 gr3         6                 +b(I,J,K,3)*(p(I+1,J,K+1)-p(I-1,J,K+1)
231.    1 MG g 4 gr3         7                 -p(I+1,J,K-1)+p(I-1,J,K-1))
232.    1 MG g 4 gr3         8                 +c(I,J,K,1)*p(I-1,J,K)+c(I,J,K,2)*p(I,J-1,K)
233.    1 MG g 4 gr3         9                 +c(I,J,K,3)*p(I,J,K-1)+wrk1(I,J,K)
234.    1 MG g 4 gr3                      SS=(S0*a(I,J,K,4)-p(I,J,K))*bnd(I,J,K)
235.    1 MG g 4 gr3                      WGOSA=WGOSA+SS*SS
236.    1 MG g 4 gr3                      wrk2(I,J,K)=p(I,J,K)+OMEGA *SS
237.                 r3-->                enddo
238.                 ---->             enddo
239.    1 MG g------->>             enddo
```

```
240.    1               C
241.  + 1 2-----------<           DO K=2,kmax-1
242.  + 1 2 3---------<              DO J=2,jmax-1
243.    1 2 3 A-------<                 DO I=2,imax-1
244.    1 2 3 A                            p(I,J,K)=wrk2(I,J,K)
245.    1 2 3 A------->                 enddo
246.    1 2 3--------->              enddo
247.    1 2----------->           enddo
248.    1               C
249.  + 1 E----------<>           call sendp(ndx,ndy,ndz).   ! P halo exchange
250.    1               C
251.  + 1                        call mpi_allreduce(wgosa,
252.    1                    >                      gosa,
253.    1                    >                      1,
254.    1                    >                      mpi_real4,
255.    1                    >                      mpi_sum,
256.    1                    >                      mpi_comm_world,
257.    1                    >                      ierr)
258.    1               C
259.    1------------->        enddo
260.                    CC End of iteration
```

Table 1: Profile by Function Group and Function

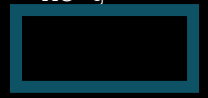
Time%	Time	Imb. Time	Imb. Time%	Calls	Group Function PE=HIDE Thread=HIDE
100.0%	6.289939	--	--	2,091.0	Total
72.5%	4.558013	--	--	384.0	OACC
55.7%	3.502276	0.043724	1.6%	93.0	jacobi_.ACC_COPY@li.212
12.5%	0.787380	0.021668	3.6%	6.0	jacobi_.ACC_COPY@li.89
3.8%	0.236862	0.005840	3.2%	93.0	jacobi_.ACC_COPY@li.238
0.4%	0.023946	0.005695	25.6%	93.0	jacobi_.ACC_SYNC_WAIT@li.238
0.1%	0.006408	0.001959	31.2%	93.0	jacobi_.ACC_ASYNC_KERNEL@li.212
0.0%	0.000692	0.000102	17.2%	3.0	jacobi_.ACC_SYNC_WAIT@li.89
0.0%	0.000450	0.000134	30.6%	3.0	jacobi_.ACC_ASYNC_KERNEL@li.89
21.5%	1.353529	--	--	99.0	USER
18.0%	1.129580	0.024657	2.8%	1.0	himenobmtxp_
2.0%	0.124014	0.008535	8.6%	1.0	initmt_
1.6%	0.098615	0.016419	19.0%	1.0	jacobi_
0.0%	0.001281	0.000173	15.8%	93.0	jacobi_.ACC_REGION@li.212
0.0%	0.000039	0.000009	25.2%	3.0	jacobi_.ACC_REGION@li.89
4.4%	0.277157	--	--	430.0	ETC
4.4%	0.276967	0.000226	0.1%	17.0	_STOP3
0.0%	0.000121	0.000013	12.6%	10.0	cuEGLApiInit
0.0%	0.000057	0.000048	60.8%	400.0	__libc_csu_init
0.0%	0.000008	0.000001	15.5%	1.0	cudbgMain
0.0%	0.000005	0.000001	19.9%	2.0	cuVDPAUCtxCreate
1.5%	0.091650	--	--	1,076.0	MPI
1.1%	0.071594	0.054624	57.7%	192.0	MPI_WAITALL
0.2%	0.014993	0.002644	20.0%	384.0	MPI_ISEND
0.1%	0.004539	0.000897	22.0%	384.0	MPI_IRECV
0.0%	0.000397	0.000015	4.9%	97.0	MPI_ALLREDUCE
0.0%	0.000053	0.000003	6.7%	1.0	MPI_CART_CREATE

Complications with Himeno

- All Arrays are in COMMON blocks – need to be global
- Reveal is putting data transfer inside the iteration loop
  - However, it does recognize that on P and WRK2 need to be updated
- Biggest issue is transferring the entire P array when only boundaries need to be exchanged
- Following charts give some optimizations for himeno that do not deal with halo exchange of P
  - The plan is to put all the arrays and operations on those arrays on the accelerator.
  - Whenever the host needs to do something with the accelerator data, we must update the host from the accelerator

Intialize arrays on the accelerator

```
148.                    C*************************************************************
149.                          subroutine initmt(mz,it)
150.                    C*************************************************************
151.                          IMPLICIT REAL*4(a-h,o-z)
152.                    C
153.                          include 'param.h'
154.                    C
155.  +                 !$OMP TARGET  DATA map(alloc:a,b,c,bnd,wrk1,wrk2,p)
156.  + MG-------------< !$OMP target teams distribute
157.    MG g-----------<       do k=1,mkmax
158.  + MG g C---------<          do j=1,mjmax
159.    MG g C gCr2-----<             do i=1,mimax
160.    MG g C gCr2                      a(i,j,k,1)=0.0
161.    MG g C gCr2                      a(i,j,k,2)=0.0
162.    MG g C gCr2                      a(i,j,k,3)=0.0
163.    MG g C gCr2                      a(i,j,k,4)=0.0
164.    MG g C gCr2                      b(i,j,k,1)=0.0
165.    MG g C gCr2                      b(i,j,k,2)=0.0
166.    MG g C gCr2                      b(i,j,k,3)=0.0
167.    MG g C gCr2                      c(i,j,k,1)=0.0
168.    MG g C gCr2                      c(i,j,k,2)=0.0
169.    MG g C gCr2                      c(i,j,k,3)=0.0
170.    MG g C gCr2 A--<>                p(i,j,k)=0.0
171.    MG g C gCr2 A--<>                wrk1(i,j,k)=0.0
172.    MG g C gCr2 A--<>                wrk2(i,j,k)=0.0
173.    MG g C gCr2 A--<>                bnd(i,j,k)=0.0
174.    MG g C gCr2----->             enddo
175.    MG g C---------->          enddo
176.    MG g---------->>       enddo
```



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```
206.                        subroutine jacobi(nn,gosa)
207.                     C***********************************************************
208.                        IMPLICIT REAL*4(a-h,o-z)
209.                     C
210.                        include 'mpif.h'
211.                        include 'param.h'
212.                     C
213.   + 1---------------<  DO loop=1,nn
214.     1                    gosa=0.0
215.     1                    wgosa=0.0
216.   + 1                !$OMP TARGET DATA map(tofrom:p)
217.     1                !  Directive inserted by Cray Reveal.  May be incomplete.
218.   + 1 MG------------< !$OMP  target teams distribute
219.     1 MG             !$OMP& private(i, j, k, s0, ss)
220.     1 MG             !$OMP& firstprivate(imax, jmax, kmax, omega)
221.     1 MG             !$OMP& map(tofrom: wgosa)
222.     1 MG             !$OMP& reduction(+: wgosa)
223.     1 MG g----------<       DO K=2,kmax-1
224.   + 1 MG g 4--------<          DO J=2,jmax-1
225.     1 MG g 4 gr3----<             DO I=2,imax-1
226.     1 MG g 4 gr3                    S0=a(I,J,K,1)*p(I+1,J,K)+a(I,J,K,2)*p(I,J+1,K)
227.     1 MG g 4 gr3          1               +a(I,J,K,3)*p(I,J,K+1)
228.     1 MG g 4 gr3          2               +b(I,J,K,1)*(p(I+1,J+1,K)-p(I+1,J-1,K)
229.     1 MG g 4 gr3          3               -p(I-1,J+1,K)+p(I-1,J-1,K))
230.     1 MG g 4 gr3          4               +b(I,J,K,2)*(p(I,J+1,K+1)-p(I,J-1,K+1)
231.     1 MG g 4 gr3          5               -p(I,J+1,K-1)+p(I,J-1,K-1))
232.     1 MG g 4 gr3          6               +b(I,J,K,3)*(p(I+1,J,K+1)-p(I-1,J,K+1)
233.     1 MG g 4 gr3          7               -p(I+1,J,K-1)+p(I-1,J,K-1))
234.     1 MG g 4 gr3          8               +c(I,J,K,1)*p(I-1,J,K)+c(I,J,K,2)*p(I,J-1,K)
235.     1 MG g 4 gr3          9               +c(I,J,K,3)*p(I,J,K-1)+wrk1(I,J,K)
236.     1 MG g 4 gr3                    SS=(S0*a(I,J,K,4)-p(I,J,K))*bnd(I,J,K)
237.     1 MG g 4 gr3                    WGOSA=WGOSA+SS*SS
238.     1 MG g 4 gr3                    wrk2(I,J,K)=p(I,J,K)+OMEGA *SS
239.     1 MG g 4 gr3----->           enddo
240.     1 MG g 4-------->         enddo
241.     1 MG g---------->>      enddo
```

```
242.    1                C
243.  + 1 MG-------------< !$OMP  target teams distribute
244.    1 MG              !$OMP& private(i, j, k)
245.    1 MG              !$OMP& firstprivate(imax, jmax, kmax)
246.    1 MG g----------<          DO K=2,kmax-1
247.  + 1 MG g 4--------<             DO J=2,jmax-1
248.    1 MG g 4 g------<                DO I=2,imax-1
249.    1 MG g 4 g                          p(I,J,K)=wrk2(I,J,K)
250.    1 MG g 4 g------>                enddo
251.    1 MG g 4-------->             enddo
252.    1 MG g--------->>          enddo
253.    1                C
254.    1                !$OMP END TARGET DATA
255.  + 1 E------------<>          call sendp(ndx,ndy,ndz)
256.    1                C
257.  + 1                          call mpi_allreduce(wgosa,
258.    1                     >                       gosa,
259.    1                     >                       1,
260.    1                     >                       mpi_real4,
261.    1                     >                       mpi_sum,
262.    1                     >                       mpi_comm_world,
263.    1                     >                       ierr)
264.    1                C
265.    1--------------->       enddo
266.                     CC End of iteration
267.                           return
268.                           end
```

At this point I am moving to illustrate halo exchanges on a different application – leslie3d

- Himeno uses MPI message types which are more confusing

- Leslie3d packs and unpacks buffers and it is easier to illustrate optimizing on the GPU

One of the eight buffers required for 3-D application

```
      IF(NCY .LT. NPY .OR. (NCY .EQ. NPY .AND. JPERIODIC)) THEN
         JCNT = 0
         DO K = 1-NLEVELS, KCMAX+NLEVELS
            DO J = JCMAX-NLEVELS+1, JCMAX
               DO I = 1-NLEVELS, ICMAX+NLEVELS
                  JCNT = JCNT + 1
                  S_N(JCNT) = VAR(I,J,K)
               END DO
            ENDDO
         END DO
         CALL MPI_SEND(S_N,
     >                 NLEVELS * NSIZE1 * NSIZE3,
     >                 MPI_DOUBLE_PRECISION,
     >                 NORTH,
     >                 MSGFLAG + MSGTSN,
     >                 MPI_COMM_WORLD,
     >                 IERR )
         IF ( IERR .NE. 0 ) CALL EJECT ('MPI_SEND FAILED: S_N')
      EN
```

Need to pack buffers on the accelerator

Packing on the GPU and sending the halo

```
738.                      #ifdef OMP_TARGET
739.    G-----------------< !$omp target teams distribute
740.    G                 #endif
741.    G g-------------<          DO K = 1, NLEVELS
742.  + G g 3-----------<             DO J = 1-NLEVELS, JCMAX+NLEVELS
743.    G g 3             #ifdef OMP_TARGET
744.  + G g 3             !$omp parallel do private(kcnt) private(i)
745.    G g 3             #endif
746.    G g 3 g---------<                 DO I = 1-NLEVELS, ICMAX+NLEVELS
747.    G g 3 g                              KCNT = (k-1)*(JCMAX+2*NLEVELS)*(ICMAX+2*NLEVELS)
748.    G g 3 g                   >                     +(j-1+NLEVELS)*(ICMAX+2*NLEVELS)+i
749.    G g 3 g                              S_I(KCNT) = VAR(I,J,K)
750.    G g 3 g--------->                 END DO
751.    G g 3----------->                ENDDO
752.    G g------------->              END DO
753.    G                 #ifdef OMP_TARGET
754.    G---------------> !$omp end target teams distribute
755.                      !$omp target update from(S_I)
756.                      #endif
757.  +                           CALL MPI_SEND(S_I,
758.                           >                NLEVELS * NSIZE1 * NSIZE2,
759.                           >                MPI_DOUBLE_PRECISION,
760.                           >                IN,
761.                           >                MSGFLAG + MSGTSI,
762.                           >                MPI_COMM_WORLD,
763.                           >                IERR )
764.  +                            IF ( IERR .NE. 0 ) CALL EJECT ('MPI_SEND FAILED: S_I')
765.                             END IF
```

We do have to update the host prior to the MPI_SEND

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Posting the receive on the Host

We don’t have to do anything prior to or after the IRECV

```
706.
707.                          IF(NCZ .GT.   1 .OR. (NCZ .EQ.   1 .AND. KPERIODIC)) THEN
708.  +                          CALL MPI_IRECV(R_I,
709.                         >                  NLEVELS * NSIZE1 * NSIZE2,
710.                         >                  MPI_DOUBLE_PRECISION,
711.                         >                  IN,
712.                         >                  MSGFLAG + MSGTRI,
713.                         >                  MPI_COMM_WORLD,
714.                         >                  MSGIDRI,
715.                         >                  IERR )
```


Receiving and unpacking on the GPU

```
785.  +                          CALL MPI_WAIT( MSGIDRI, MPI_STATUS, IERR)
786.
787.                       #ifdef OMP_TARGET
788.                       !$omp target update to(R_I)
789.    G---------------< !$omp target teams distribute
790.    G                 #endif
791.    G g-------------<          DO K = 1-NLEVELS, 0
792.  + G g 3-----------<             DO J = 1-NLEVELS, JCMAX+NLEVELS
793.    G g 3             #ifdef OMP_TARGET
794.  + G g 3             !$omp parallel do private(kcnt) private(i)
795.    G g 3             #endif
796.    G g 3 g---------<                DO I = 1-NLEVELS, ICMAX+NLEVELS
797.    G g 3 g                           KCNT = (k-1+NLEVELS)*(JCMAX+2*NLEVELS)*(ICMAX+2*NLEVELS)
798.    G g 3 g                 >                          +(j-1+NLEVELS)*(ICMAX+2*NLEVELS)+i
799.    G g 3 g                             VAR(I,J,K) = R_I(KCNT)
800.    G g 3 g--------->                END DO
801.    G g 3----------->             END DO
802.    G g------------->          END DO
803.    G                 #ifdef OMP_TARGET
804.    G---------------> !$omp end target teams distribute
805.                      #endif
```

After the MPI_WAIT we need to update the GPU with the communicated array

Still can do better – use use_device_ptr and setenv MPICH_RDMA_ENABLED_CUDA 1

```
#ifdef OMP_TARGET
!$omp target enter data map(to:VAR)
!$omp&          map(alloc:R_N,R_W,R_S,R_E,R_I,R_O,S_N,S_W,S_S,
!$OMP&                  S_E,S_I,S_O)
!$omp target data
!$omp&  use_device_ptr(R_N,R_W,R_S,R_E,R_I,R_O,S_N,S_W,S_S,
!$OMP&                  S_E,S_I,S_O)
#endif

      CALL MPI_IRECV(R_W,
     >               NLEVELS * NSIZE2 * NSIZE3,
     >               MPI_DOUBLE_PRECISION,
     >               WEST,
     >               MSGFLAG + MSGTRW,
     >               MPI_COMM_WORLD,
     >               MSGIDRW,
     >               IERR)
```

Much easier to code –

Do not need target update clauses

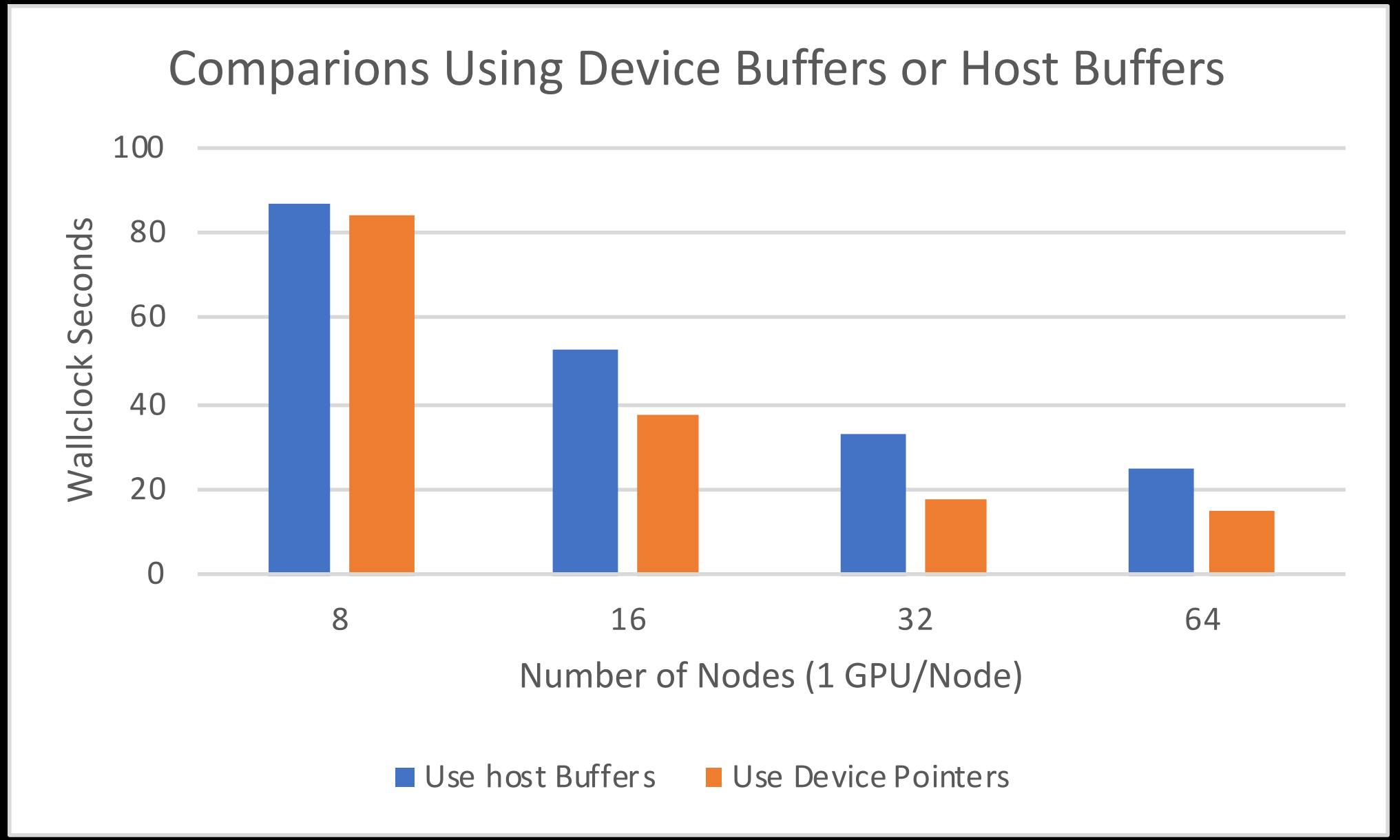
Still can do better

```
  ifdef OMP_TARGET
!$omp target enter data map(to:VAR)
!$omp&          map(alloc:R_N,R_W,R_S,R_E,R_I,R_O,S_N,S_W,S_S,
!$OMP&                  S_E,S_I,S_O)
!$omp target data
!$omp&  use_device_ptr(R_N,R_W,R_S,R_E,R_I,R_O,S_N,S_W,S_S,
!$OMP&                  S_E,S_I,S_O)
#endif
```

```
      CALL MPI_SEND(S_E,
     >              NLEVELS * NSIZE2 * NSIZE3,
     >              MPI_DOUBLE_PRECISION,
     >              EAST,
     >              MSGFLAG + MSGTSE,
     >              MPI_COMM_WORLD,
     >              IERR )
```

Much easier to code

All Packing done on the GPU



CRAY_ACC_DEBUG Environment Variable

- Three levels of verbosity
  - 1 High Level overview of kernels executed and data transferred
  - 2 Breaks down data transfer by each variable
  - 3 The whole Kitchen sink

setenv CRAY_ACC_DEBUG 1

```
ACC: Transfer 29 items (to acc 0 bytes, to host 0 bytes) from src/fluxi.f:21
ACC: Transfer 15 items (to acc 0 bytes, to host 0 bytes) from src/fluxi.f:114
ACC: Transfer 1 items (to acc 0 bytes, to host 0 bytes) from src/fluxi.f:141
ACC: Transfer 29 items (to acc 0 bytes, to host 0 bytes) from src/fluxi.f:21
ACC: Transfer 15 items (to acc 0 bytes, to host 0 bytes) from src/fluxi.f:114
ACC: Transfer 1 items (to acc 0 bytes, to host 0 bytes) from src/fluxi.f:141
ACC: Execute kernel extrapi_$ck_L141_7 async(auto) from src/fluxi.f:141
ACC: Execute kernel extrapi_$ck_L141_7 async(auto) from src/fluxi.f:141
ACC: Wait async(auto) from src/fluxi.f:172
ACC: Transfer 1 items (to acc 0 bytes, to host 0 bytes) from src/fluxi.f:172
ACC: Execute kernel extrapi_$ck_L173_9 async(auto) from src/fluxi.f:173
ACC: Wait async(auto) from src/fluxi.f:172
```


setenv CRAY_ACC_DEBUG 2

```
ACC: Start transfer 29 items from src/fluxi.f:21
ACC:         present 'dq' (255923712 bytes)
ACC:         present 'ds' (95971392 bytes)
ACC:         present 'ds1' (95971392 bytes)
ACC:         present 'dtv' (31990464 bytes)
ACC:         present 'hf' (127961856 bytes)
ACC:         present 'pav' (31990464 bytes)
ACC:         present 'q' (511847424 bytes)
ACC:         present 'qav' (255923712 bytes)
ACC:         present 'six' (31990464 bytes)
ACC:         present 'siy' (31990464 bytes)
ACC:         present 'siz' (31990464 bytes)
ACC:         present 't' (31990464 bytes)
```

setenv CRAY_ACC_DEBUG 3

```
ACC: Start transfer 29 items from src/fluxi.f:21
ACC:   flags: RETURN_ACC_TIME
ACC:
ACC:   Trans 1
ACC:       Simple transfer of 'dq' (144 bytes)
ACC:            host ptr 78b538
ACC:            acc  ptr 0
ACC:            flags: DOPE_VECTOR DV_ONLY_DATA ALLOCATE COPY_HOST_TO_ACC ACQ_PRESENT REG_PRESENT
ACC:            Transferring dope vector
ACC:              dim:1 lowbound:-2 extent:198 stride_mult:1
ACC:              dim:2 lowbound:-2 extent:198 stride_mult:198
ACC:              dim:3 lowbound:-2 extent:102 stride_mult:39204
ACC:              dim:4 lowbound:1 extent:8 stride_mult:3998808
ACC:              DV size=255923712 (scale:8, elem_size:8)
ACC:              total mem size=255923712 (dv:0 obj:255923712)
ACC:            host region 4dac8780 to 5ced9d80 found in present table index 0 (ref count 2)
ACC:            memory found in present table (2aaaf2000000, base 2aaaf2000000)
ACC:            new acc ptr 2aaaf2000000
```


So what have we learned

- Perftools is excellent for identifying issues in existing applications for improving threading, vectorization and scalar optimization
- Reveal can help with the difficult job of scoping variables in potential parallelizable loops
  - More difficult if not impossible with C++
- Moving to the GPU is difficult; however, it can be done in steps that are more manageable
  - Perftools identifies the bottlenecks in the GPU application very quickly
- GPU direct is best way to do the message passing – in this case it only matters at scale

Thank you