Preparing an application for Hybrid Supercomputing using Cray's Tool Suite

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Systems and Software being used

- Using 4-8 Intel Broadwell nodes – 44 cores/node
- Also using cce/9.0.0.23676 and cray-accel-nvidia60
- Perftools-base/7.1.0
- Using four nodes with 1 P100s on each node for first set of runs
- Using up to 512 nodes with P100s on each node for scaling runs

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

Perftools-lite profile – Run on 8 nodes–1 MPI task/node

```
Table 1:  Profile by Function


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


 100.0% | 4,061.6 |   -- |    -- | Total
|-----------------------------------------------
|  95.0% | 3,859.9 |   -- |    -- | USER
||----------------------------------------------
||  21.4% |   869.6 |  8.4 |  1.1% | fluxj_
||  20.7% |   842.8 |  7.2 |  1.0% | fluxi_
||  19.9% |   808.2 |  5.8 |  0.8% | fluxk_
||   7.9% |   318.9 |  6.1 |  2.2% | extrapk_
||   7.5% |   303.2 |  7.8 |  2.8% | extrapi_
||   6.8% |   274.2 |  3.8 |  1.5% | update_
||   6.1% |   249.4 |  4.6 |  2.1% | extrapj_
||   1.0% |    40.5 |  5.5 | 13.7% | mpicx_
||==============================================
|   4.1% |   165.2 |   -- |    -- | MPI
||----------------------------------------------
||   2.2% |    91.1 |  5.9 |  6.9% | MPI_REDUCE
||   1.1% |    44.9 | 31.1 | 46.8% | MPI_SEND
|==============================================
```

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 8 nodes–8 MPI tasks

```
Table 2:  Profile by Group, Function, and Line
  Samp% |    Samp | Imb. |  Imb. | Group
        |         | Samp | Samp% |  Function=[MAX10]
        |         |      |       |   Source
        |         |      |       |    Line
        |         |      |       |     PE=HIDE

 100.0% | 4,061.6 |   -- |    -- | Total
|-----------------------------------------------------------------------
|  95.0% | 3,859.9 |   -- |    -- | USER
||----------------------------------------------------------------------
||  21.4% |   869.6 |   -- |    -- | fluxj_
3|        |         |      |       |  Leslie_CUG/leslie3d_mpi/src/fluxj.f
||||--------------------------------------------------------------------
4|||   1.6% |    63.6 |  8.4 | 13.3% | line.31
4|||  14.0% |   567.5 | 15.5 |  3.0% | line.67
4|||   2.7% |   109.6 | 12.4 | 11.6% | line.76
||||====================================================================
||  20.7% |   842.8 |   -- |    -- | fluxi_
3|        |         |      |       |  Leslie_CUG/leslie3d_mpi/src/fluxi.f
||||--------------------------------------------------------------------
4|||   1.9% |    77.1 | 18.9 | 22.5% | line.24
4|||  14.2% |   578.8 | 21.2 |  4.0% | line.56
4|||   2.1% |    85.5 | 10.5 | 12.5% | line.63
||||====================================================================
||  19.9% |   808.2 |   -- |    -- | fluxk_
3|        |         |      |       |  Leslie_CUG/leslie3d_mpi/src/fluxk.f
||||--------------------------------------------------------------------
4|||   1.7% |    69.0 | 13.0 | 18.1% | line.31
4|||  12.2% |   497.5 | 21.5 |  4.7% | line.65
4|||   3.2% |   129.6 | 18.4 | 14.2% | line.74
```

Profile on line level within a routine – lets look at this routine

Perftools-lite profile – Run on 8 nodes–8 MPI tasks

```
28.  + F------------------<       DO K = 1, KCMAX
29.  + F F----------------<          DO J = 0, JCMAX
30.    F F V------------- <            DO I = 1, IND
31.    F F V                          QS(I) = UAV(I,J,K) * SJX(I,J,K) +
32.    F F V                  >                VAV(I,J,K) * SJY(I,J,K) +
33.    F F V                  >                WAV(I,J,K) * SJZ(I,J,K)
34.    F F V
35.    F F V                           IF (NSCHEME .EQ. 2) THEN
36.    F F V                              L = J + 1 - JADD
37.    F F V
38.    F F V                                 QSP = U(I,L,K) * SJX(I,J,K) +
39.    F F V                  >                    V(I,L,K) * SJY(I,J,K) +
40.    F F V                  >                    W(I,L,K) * SJZ(I,J,K)
41.    F F V                                 QSPJ = (QSP - QS(I)) * DBLE(1 - 2 * JADD)
42.    F F V                                 IF (QSPJ .GT. 0.0D+00) QS(I) = 0.5D+00 * (QS(I) + QSP)
43.    F F V
44.    F F V                           ENDIF
45.    F F V
46.    F F V                          FSJ(I,J,1) =  QAV(I,J,K,1) * QS(I)
47.    F F V                          FSJ(I,J,2) =  QAV(I,J,K,2) * QS(I) +
48.    F F V                  >                     PAV(I,J,K) * SJX(I,J,K)
49.    F F V                          FSJ(I,J,3) =  QAV(I,J,K,3) * QS(I) +
50.    F F V                  >                     PAV(I,J,K) * SJY(I,J,K)
51.    F F V                          FSJ(I,J,4) =  QAV(I,J,K,4) * QS(I) +
52.    F F V                  >                     PAV(I,J,K) * SJZ(I,J,K)
53.    F F V                          FSJ(I,J,5) = (QAV(I,J,K,5) + PAV(I,J,K)) *
54.    F F V                  >                                          QS(I)
55.    F F V
56.    F F V                          IF (ISGSK .EQ. 1) THEN
57.    F F V                             FSJ(I,J,7) = QAV(I,J,K,7) * QS(I)
58.    F F V                          ENDIF
59.    F F V
60.    F F V                          IF ( ICHEM .GT. 0 ) THEN
61.    F F V D------------<              DO L = 8, 7 + NSPECI
62.    F F V D                             FSJ(I,J,L) = QAV(I,J,K,L) * QS(I)
63.    F F V D------------>              ENDDO
64.    F F V                          ENDIF
65.    F F V--------------->       ENDDO
66.    F F
67.  + F F V I-----------<>           IF ( VISCOUS ) CALL VISCJ (1, IND, J, K, FSJ)
68.    F F---------------->        ENDDO
```

+ indicates further information

You get this listing by using –hlist-a

Line 67 from –hlist=a

I indicates the call was inlined , V loop Vectorized, F Flattened

Perftools-lite profile – Run on 8 nodes–8 MPI tasks

```
ftn-6315 ftn: VECTOR FLUXJ, File = fluxj.f, Line = 28
  A loop starting at line 28 was not vectorized because the target array (qs) would require rank expansion.


ftn-3182 ftn: IPA FLUXJ, File = fluxj.f, Line = 28, Column = 7
  Loop has been flattened.


ftn-6315 ftn: VECTOR FLUXJ, File = fluxj.f, Line = 29
  A loop starting at line 29 was not vectorized because the target array (qs) would require rank expansion.


ftn-3182 ftn: IPA FLUXJ, File = fluxj.f, Line = 29, Column = 10
  Loop has been flattened.


ftn-6204 ftn: VECTOR FLUXJ, File = fluxj.f, Line = 30
  A loop starting at line 30 was vectorized.


ftn-6002 ftn: SCALAR FLUXJ, File = fluxj.f, Line = 61
  A loop starting at line 61 was eliminated by optimization.


ftn-6383 ftn: VECTOR FLUXJ, File = fluxj.f, Line = 67
  A loop starting at line 67 requires an estimated 25 vector registers at line 67; 2 of these have been preemptively forced to
  memory.


ftn-6204 ftn: VECTOR FLUXJ, File = fluxj.f, Line = 67
  A loop starting at line 67 was vectorized.
```

Perftools-lite profile – Run on 8 nodes–8 MPI tasks

```
Table 1:  Function Calltree View
  Samp% |    Samp | Calltree
        |         |  PE=HIDE
 100.0% | 4,061.6 | Total
|-----------------------------------
|  85.1% | 3,456.6 | les3d_
||----------------------------------
||  27.8% | 1,127.1 | fluxk_
|||---------------------------------
3||  19.9% |   808.2 | fluxk_(exclusive)
3||   7.9% |   318.9 | extrapk_
|||=================================
||  27.6% | 1,119.0 | fluxj_
|||---------------------------------
3||  21.4% |   869.6 | fluxj_(exclusive)
3||   6.1% |   249.4 | extrapj_
|||=================================
||  20.7% |   842.8 | fluxi_
||   2.8% |   115.4 | parallel_
3|   2.1% |    87.0 |  mpicx_
||||-------------------------------
4|||   1.1% |    44.9 | MPI_SEND
4|||   1.0% |    40.5 | mpicx_(exclusive)
||||===============================
||   2.3% |    92.0 | flowio_
3|   2.2% |    91.1 |  MPI_REDUCE
||   1.1% |    45.9 | tmstep_
||=================================
|   7.5% |   303.2 | extrapi_
|   6.8% |   274.2 | update_
```

Pat_report –Oct <statistics directory>

Level in the Call Tree, everything 3 and higher is called from this || (2)

Perftools-lite-loops – Run on 8 nodes–8 MPI tasks

Table 1: Inclusive and Exclusive Time in Loops (from -hprofile_generate)

Loop Incl Time%	Loop Incl Time	Loop Hit	Loop Trips Avg	Loop Trips Min	Loop Trips Max	Function=/.LOOP[.] PE=HIDE
96.9%	60.109652	1	100.0	100	100	les3d_.LOOP.3.li.216
96.0%	59.527700	100	2.0	2	2	les3d_.LOOP.4.li.272
23.3%	14.461074	200	96.0	96	96	fluxi_.LOOP.1.li.21
23.3%	14.460550	19,200	96.0	96	96	fluxi_.LOOP.2.li.22
20.5%	12.724507	200	96.0	96	96	fluxk_.LOOP.1.li.28
20.1%	12.486995	200	96.0	96	96	fluxj_.LOOP.1.li.28
15.1%	9.370239	19,200	97.0	97	97	fluxj_.LOOP.2.li.29
14.0%	8.713997	19,200	97.0	97	97	fluxk_.LOOP.2.li.29
10.1%	6.259900	1,843,200	97.0	97	97	visci_.LOOP.1.li.782
8.8%	5.445447	1,862,400	96.0	96	96	viscj_.LOOP.1.li.347
8.0%	4.990874	1,862,400	96.0	96	96	visck_.LOOP.1.li.348
7.9%	4.905076	200	97.0	97	97	extrapk_.LOOP.1.li.141
7.9%	4.904410	19,400	99.0	99	99	extrapk_.LOOP.2.li.143
7.6%	4.704280	1,843,200	96.0	96	96	fluxi_.LOOP.4.li.60
6.6%	4.121449	200	99.0	99	99	extrapj_.LOOP.1.li.141
6.6%	4.121028	19,800	97.0	97	97	extrapj_.LOOP.2.li.142
6.5%	4.009192	19,200	96.0	96	96	fluxk_.LOOP.4.li.69
6.4%	3.995474	1,843,200	96.0	96	96	fluxk_.LOOP.5.li.71
5.5%	3.382283	200	99.0	99	99	extrapi_.LOOP.1.li.123
5.5%	3.381946	19,800	99.0	99	99	extrapi_.LOOP.2.li.124
5.0%	3.115988	19,200	96.0	96	96	fluxj_.LOOP.4.li.71
5.0%	3.102463	1,843,200	96.0	96	96	fluxj_.LOOP.5.li.73

This Table shows most important loops, the columns are percent of time, inclusive time, number of times the loop was executed, Avg, Min, Max iteration counts and location within the source

How do I know what the important loops are?

- Pat_report –O calltree < directory produced by perftools-lite-loops run>

- Produces call tree with DO loops included

Perftools-lite-loops – Run on 8 nodes–8 MPI tasks

```
Table 1:  Function Calltree View
  Time% |       Time |       Calls | Calltree
        |            |             |  PE=HIDE
 100.0% | 60.437329 |          -- | Total
|-----------------------------------------------------------
| 100.0% | 60.437286 |         2.0 | les3d_
||----------------------------------------------------------
||  96.8% | 58.504830 |          -- | les3d_.LOOP.3.li.216
3|  95.8% | 57.923177 |          -- |  les3d_.LOOP.4.li.272
||||---------------------------------------------------------
4|||  30.9% | 18.681501 |       200.0 | fluxi_
|||||--------------------------------------------------------
5||||  12.1% |  7.338945 |       200.0 | fluxi_(exclusive)
```

Three FLUX routines accounting for 35% of the time

```
5||||  12.1% |  7.338945 |       200.0 | fluxi_(exclusive)
5||||  11.4% |  6.863554 |          -- | fluxi_.LOOP.1.li.21
6||||        |           |              |  fluxi_.LOOP.2.li.22
7||||  11.4% |  6.863554 | 1,843,200.0 |   visci_

5||||   9.4% |  5.654640 |          -- | fluxk_.LOOP.1.li.28
6||||        |           |              |  fluxk_.LOOP.2.li.29
7||||   9.4% |  5.654640 | 1,862,400.0 |   visck_

|||||-----------------------------------------------------
5||||  10.2% |  6.136293 |          -- | fluxj_.LOOP.1.li.28
6||||        |           |              |  fluxj_.LOOP.2.li.29
7||||  10.2% |  6.136293 | 1,862,400.0 |   viscj_
```

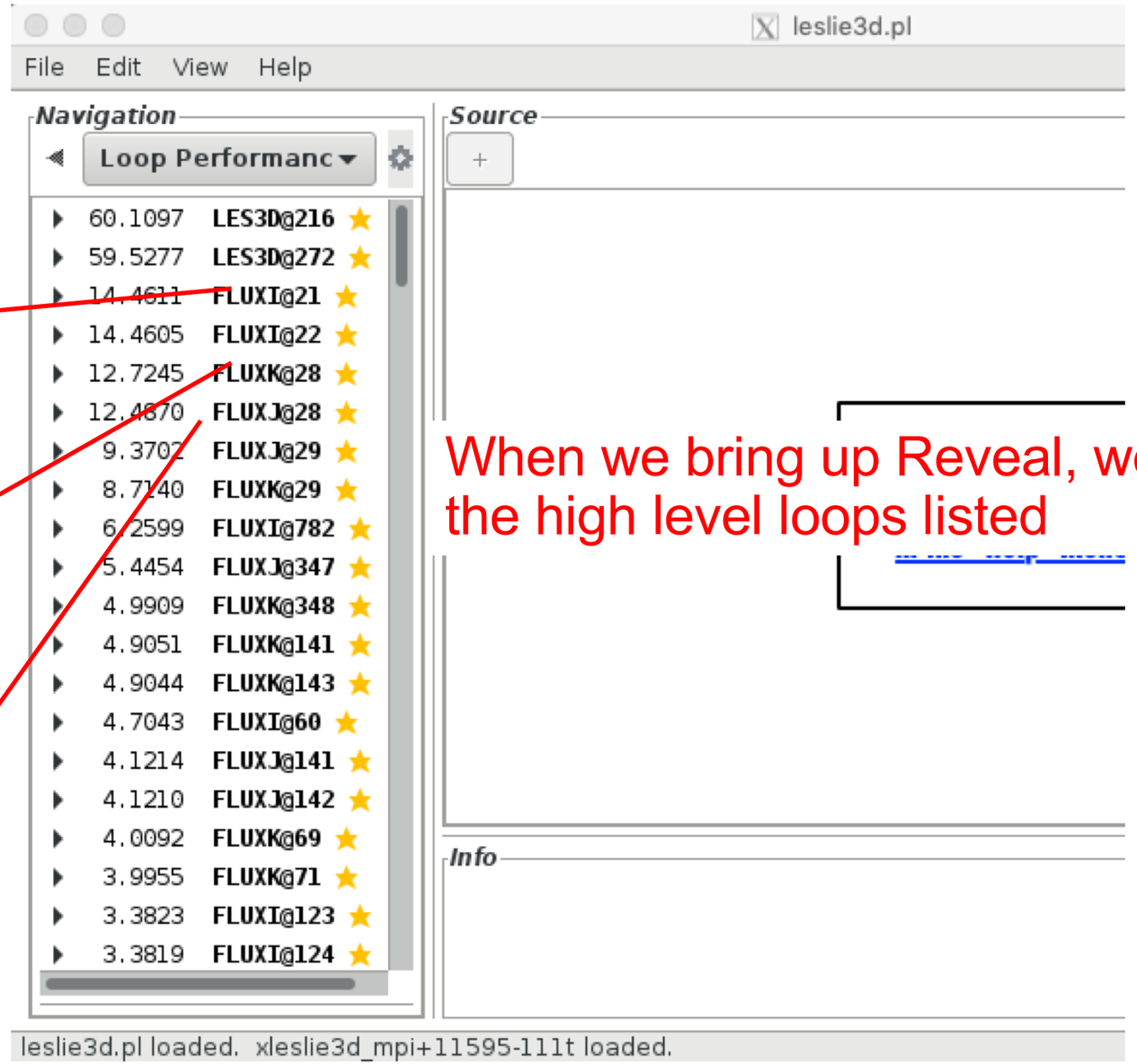
Using Reveal

- Need program library and perftools-lite-loops output
  - ftn -hlist=a –hpl=leslie3d.pl
  - reveal leslie3d.pl < perftools-lite-loops data directory>

DO NOT HAVE any PERFTOOLS-LITE or PERFTOOLS modules loaded when you build the program library

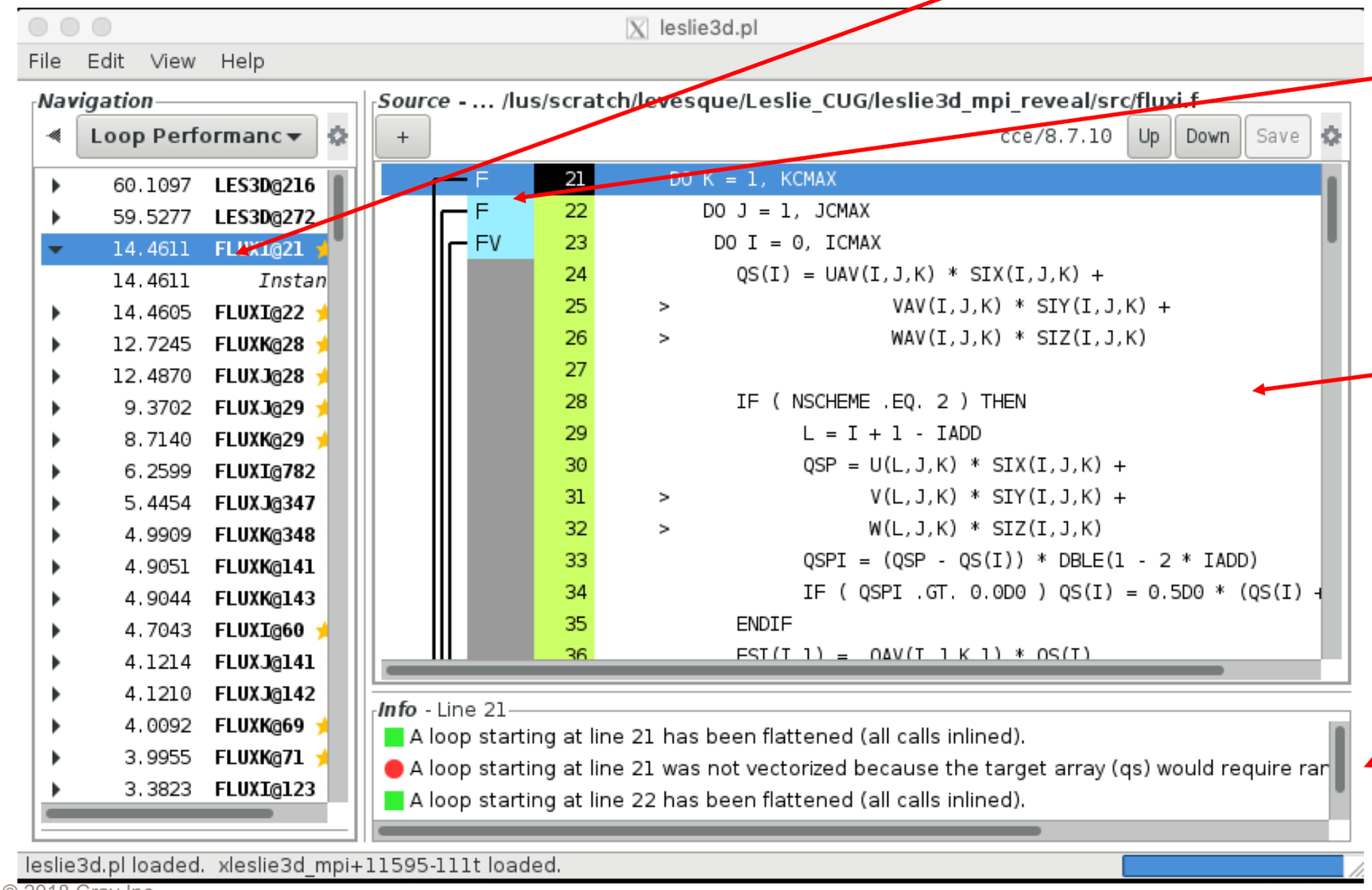
Perftools-lite-loops – Run on 8 nodes–1 MPI task/Node

```
Table 1:  Function Calltree View
  Time% |       Time |       Calls | Calltree
        |            |             |  PE=HIDE
 100.0% | 60.437329 |          -- | Total
|-----------------------------------------------------------
| 100.0% | 60.437286 |         2.0 | les3d_
||----------------------------------------------------------
||  96.8% | 58.504830 |          -- | les3d_.LOOP.3.li.216
3|  95.8% | 57.923177 |          -- |  les3d_.LOOP.4.li.272
||||---------------------------------------------------------
4|||  30.9% | 18.681501 |       200.0 | fluxi_
|||||---------------------------------------------------------
5||||  12.1% |  7.338945 |       200.0 | fluxi_(exclusive)
5||||  11.4% |  6.863554 |          -- | fluxi_.LOOP.1.li.21
6||||        |           |             |  fluxi_.LOOP.2.li.22
7||||  11.4% |  6.863554 | 1,843,200.0 |   visci_
5||||   7.4% |  4.479002 |       200.0 | extrapi_
||||||--------------------------------------------------------
6|||||   3.8% |  2.320974 |       200.0 | extrapi_(exclusive)
6|||||   3.6% |  2.158027 |          -- | extrapi_.LOOP.1.li.123
7|||||       |           |             |  extrapi_.LOOP.2.li.124
8|||||   3.6% |  2.158027 | 1,960,200.0 |   exi4_
|||||=========================================================
4|||  28.3% | 17.098408 |       200.0 | fluxk_
|||||---------------------------------------------------------
5||||  11.3% |  6.809059 |       200.0 | fluxk_(exclusive)
5||||   9.4% |  5.654640 |          -- | fluxk_.LOOP.1.li.28
6||||        |           |             |  fluxk_.LOOP.2.li.29
7||||   9.4% |  5.654640 | 1,862,400.0 |   visck_
5||||   7.7% |  4.634709 |       200.0 | extrapk_
||||||--------------------------------------------------------
6|||||   4.9% |  2.959637 |          -- | extrapk_.LOOP.1.li.141
7|||||       |           |             |  extrapk_.LOOP.2.li.143
8|||||   4.9% |  2.937827 | 1,900,800.0 |   exk4_
6|||||   2.8% |  1.675072 |       200.0 | extrapk_(exclusive)
|||||=========================================================
4|||  26.6% | 16.077506 |       200.0 | fluxj_
|||||---------------------------------------------------------
5||||  10.2% |  6.136293 |          -- | fluxj_.LOOP.1.li.28
6||||        |           |             |  fluxj_.LOOP.2.li.29
7||||  10.2% |  6.136293 | 1,862,400.0 |   viscj_
5||||  10.1% |  6.090073 |       200.0 | fluxj_(exclusive)
5||||   6.4% |  3.851140 |       200.0 | extrapj_
```



When we bring up Reveal, we get the high level loops listed

Click on important loop – Right Click to Scope



Annotation of optimization of code

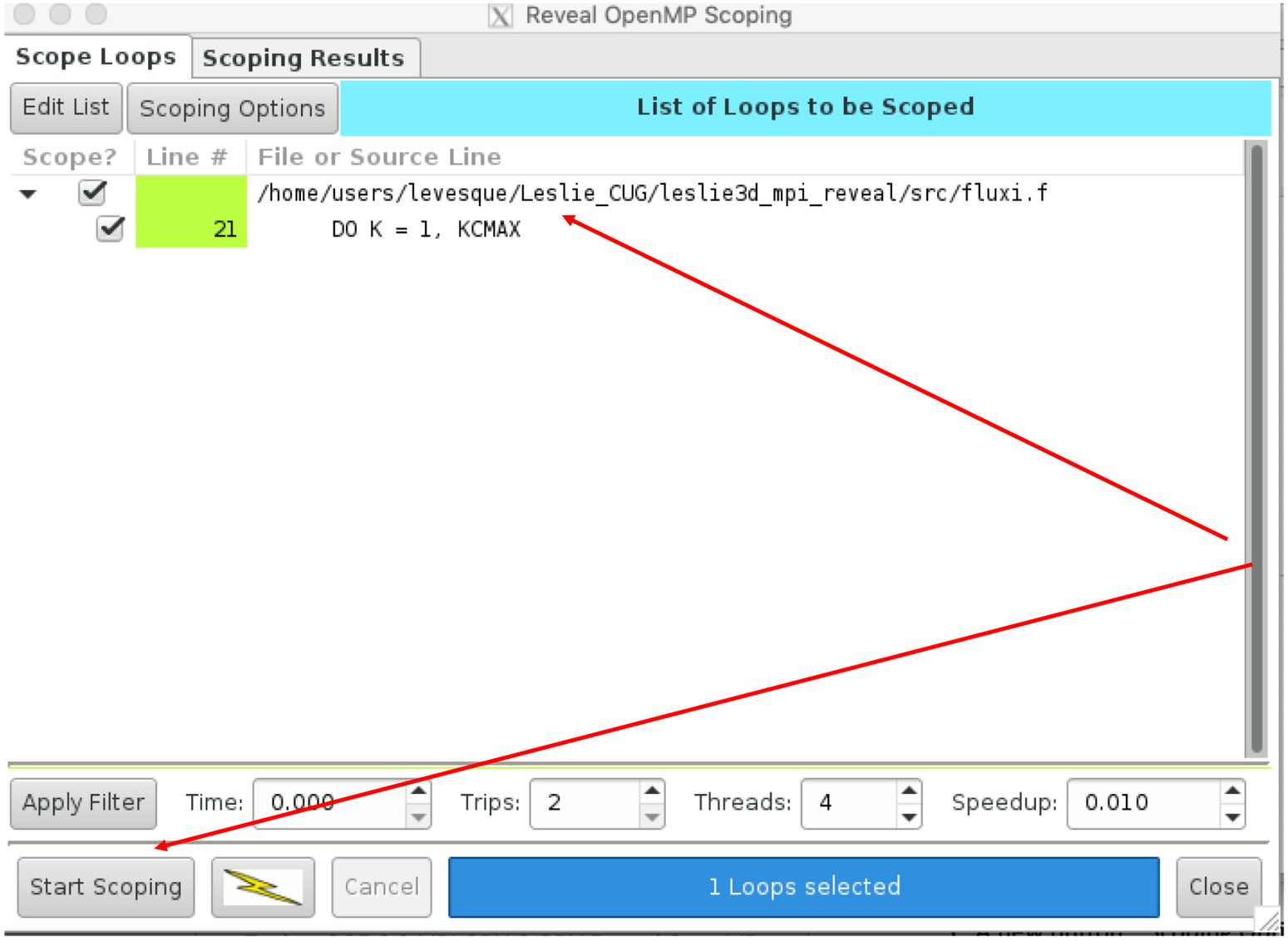
F- Flattened

V- Vectorized

Listing of loop

Diagnostics from compiler

Scoping Window



Then up pops the Scoping window

Loop selected Just click on Start Scoping

Scoping results

Array	P S C **U**	WARN: LastPrivate of array may be very expensive.
		FAIL: FirstPrivate/Shared Scope Conflict.
Scalar	P S C **U**	FAIL: Possible recurrence involving this object.
Scalar	P S C **U**	FAIL: conflicting requirements, unable to scope.
Scalar	P S C **U**	FAIL: Possible recurrence involving this object.
Array	P S C **U**	WARN: LastPrivate of array may be very expensive.
		FAIL: Last defining iteration not known for variable that may be live on exit.

P – Private

S – Shared

C – Conflict

U - Unresolved

User can now change scope by selecting the appropriate letter

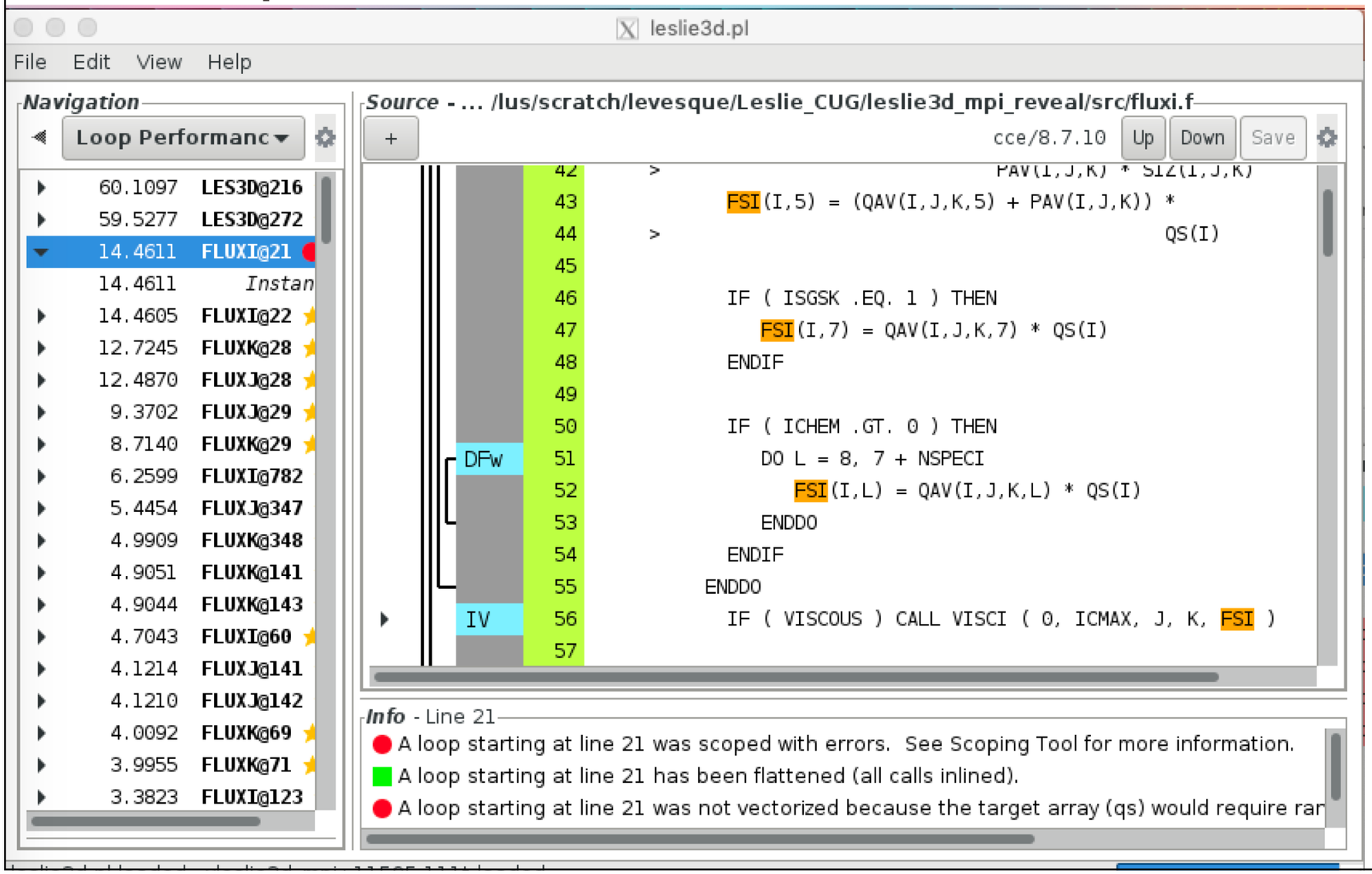
What can the user do to help Reveal

- Trace each variable that is unresolved and decide whether it is a potential race condition or can be scoped private or shared
  - If okay, make private or shared
- Once you have resolved all the unresolved variables then select the Insert Directives
- Couple definitions
  - Array Constant – An array not referenced by the parallel loop index
  - Array Constant reduction - example

With respect to K - A(I,J) is an array reduction

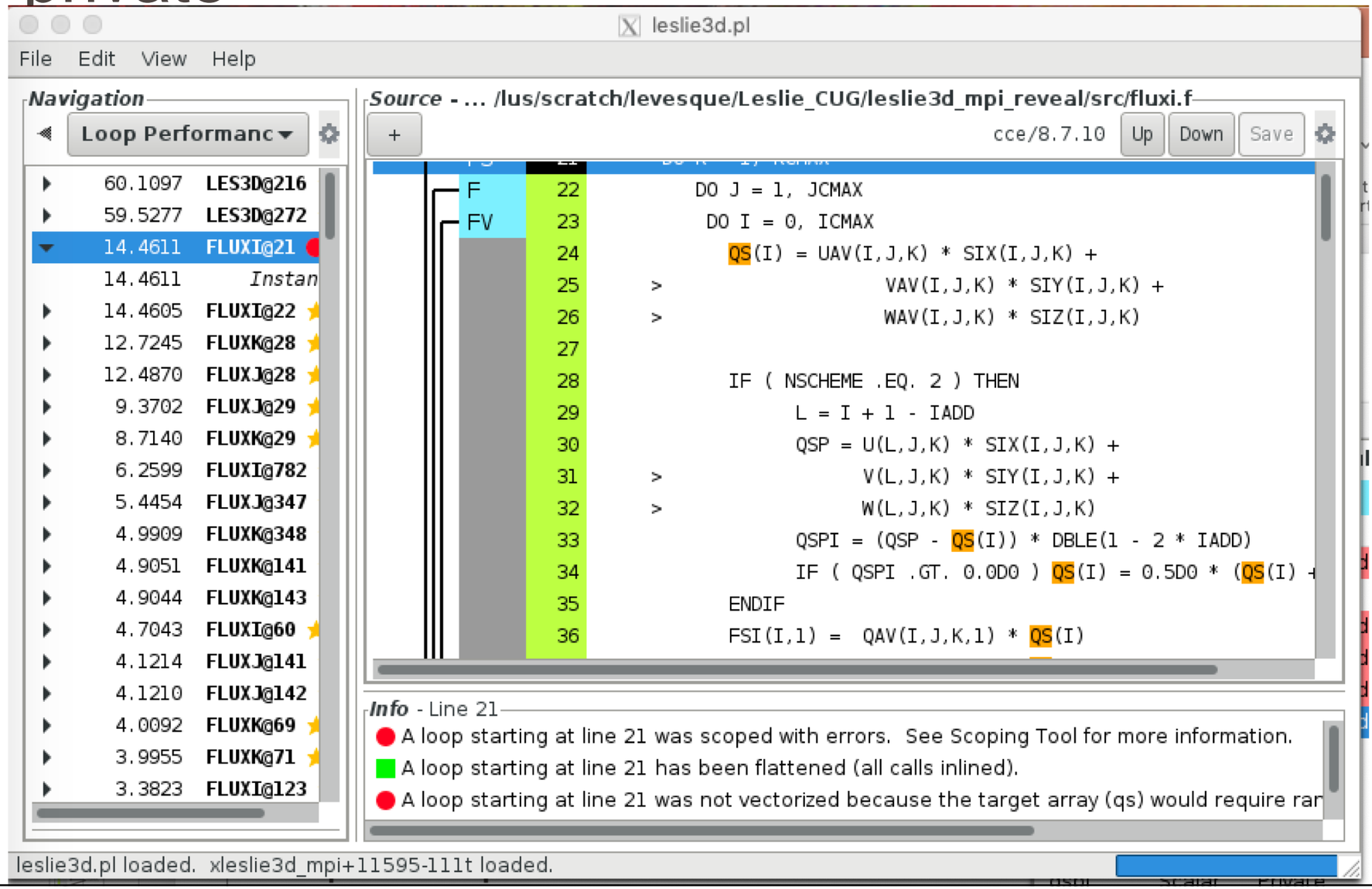
```
do j=1,n
  do I=1,n
    do k=1,n
    a(i,j) = a(i,j) + b(i,k)*c(j,k)
    enddo
  enddo
enddo
```

Array Constants are difficult to scope, especially when passed to a routine



If you select a variable in the scoping window, all occurrences are highlighted in the main window

The compiler doesn't scope either FSI or QS as private



Some Simple Scoping rules

- A scalar or an array not dependent on the loop being parallelized (array constant) should be private or ordered dependency
  - If the scalar is set prior to being used each time through the loop, then it is private. If it is not then it will result in a race condition
  - All elements of a array constant must be set prior to being used each pass through the loop. In those cases where not all the elements of the array are set prior to being used, first value getting is required.

Some Simple Scoping rules

- All arrays dependent upon the loop being parallelized should be shared. The compiler must perform data dependency analysis on the arrays to assure that there is no order dependency

- A reduction variable or constant array reduction is a special case that is identified by most compilers and must be in a reduction clause.

- Any variable that is just read is a shared variable

Complications down the call chain and modules

- No scoping directives can be inserted within those routines called from a parallelized loop.
  - All global variables must be shared
  - All variables allocated on stack must be private
- No private variables are allowed within a COMMON block or a module unless they are noted on a THREADPRIVATE directive

Lastprivate saving and Firstprivate getting

- These two issues can drive you mad
  - Last Value saving is when the last value of a private variable is used outside the parallel loop. I can say that I have seen this in about .00001 % of the applications I have looked at – very rare.
    - When you select last value saving, the compiler has to make sure that the master thread either execute the last pass through the loop or have the thread, that does the last past, copy its private variable to the master
    - Last value saving can have a big performance hit

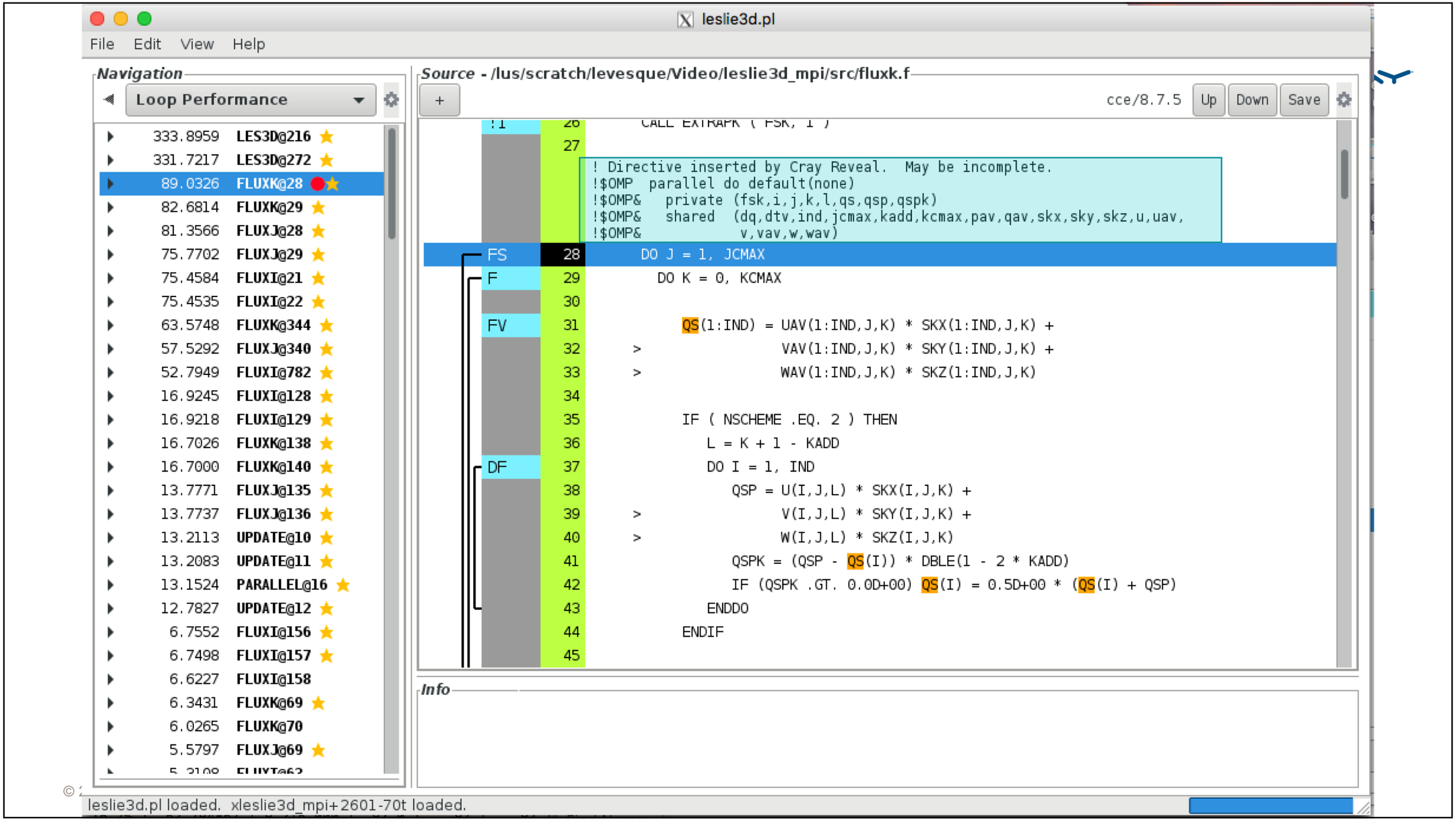
Lastprivate saving and Firstprivate getting

- These two issues can drive you mad
  - First value saving is more common. This is when the master has to copy the value of it’s private variable to all other threads. There is not much of a performance hit from doing first value saving

After analyzing the variables that are unresolved

- If you are confident of your changes and all unresolved are resolved then click on INSERT Directives
  - CAUTION – if you are wrong you will be inserting a race condition

- If you cannot confidently resolve the unresolved, then go on to another loop


leslie3d.pl
File Edit View Help
Navigation
Loop Performance
333.8959 LES3D@216
331.7217 LES3D@272
89.0326 FLUXK@28
82.6814 FLUXK@29
81.3566 FLUXJ@28
75.7702 FLUXJ@29
75.4584 FLUXI@21
75.4535 FLUXI@22
63.5748 FLUXK@344
57.5292 FLUXJ@340
52.7949 FLUXI@782
16.9245 FLUXI@128
16.9218 FLUXI@129
16.7026 FLUXK@138
16.7000 FLUXK@140
13.7771 FLUXJ@135
13.7737 FLUXJ@136
13.2113 UPDATE@10
13.2083 UPDATE@11
13.1524 PARALLEL@16
12.7827 UPDATE@12
6.7552 FLUXI@156
6.7498 FLUXI@157
6.6227 FLUXI@158
6.3431 FLUXK@69
6.0265 FLUXK@70
5.5797 FLUXJ@69
Source - /lus/scratch/levesque/Video/leslie3d_mpi/src/fluxk.f
+
cce/8.7.5
Up
Down
Save
!1 26 CALL EXTRAPK (FSK, 1)
27
! Directive inserted by Cray Reveal. May be incomplete.
!$OMP parallel do default(none)
!$OMP& private (fsk,i,j,k,l,qs,qsp,qspk)
!$OMP& shared (dq,dtv,ind,jcmax,kadd,kcmax,pav,qav,skx,sky,skz,u,uav,
!$OMP& v,vav,w,wav)
FS 28 DO J = 1, JCMAX
F 29 DO K = 0, KCMAX
30
FV 31 QS(1:IND) = UAV(1:IND,J,K) * SKX(1:IND,J,K) +
32 > VAV(1:IND,J,K) * SKY(1:IND,J,K) +
33 > WAV(1:IND,J,K) * SKZ(1:IND,J,K)
34
35 IF (NSCHEME .EQ. 2) THEN
36 L = K + 1 - KADD
DF 37 DO I = 1, IND
38 QSP = U(I,J,L) * SKX(I,J,K) +
39 > V(I,J,L) * SKY(I,J,K) +
40 > W(I,J,L) * SKZ(I,J,K)
41 QSPK = (QSP - QS(I)) * DBLE(1 - 2 * KADD)
42 IF (QSPK .GT. 0.0D+00) QS(I) = 0.5D+00 * (QS(I) + QSP)
43 ENDDO
44 ENDIF
45
Info
leslie3d.pl loaded. xleslie3d_mpi+2601-70t loaded.

Reveal helped analyze this loop

```
    28.                     ! Directive inserted by Cray Reveal.  May be incomplete.
                          ! Directive inserted by Cray Reveal.  May be incomplete.
M-----------------< !$OMP  parallel do default(none)
M                 !$OMP&   private (fsk,i,j,k,l,qs,qsp,qspk)
M                 !$OMP&   shared  (dq,dtv,ind,jcmax,kadd,kcmax,pav,qav,skx,sky,skz,u,uav,
M                 !$OMP&            v,vav,w,wav)


    38.     M mF F V              >                WAV(I,J,K) * SKZ(I,J,K)
    39.     M mF F V
    40.     M mF F V                    IF ( NSCHEME .EQ. 2 ) THEN
    41.     M mF F V                       L = K + 1 - KADD
    42.     M mF F V
    43.     M mF F V
    44.     M mF F V
    45.     M mF F V
    46.     M mF F V                          IF (QSPK .GT. 0.0D+00) QS(I) = 0.5D+00 * (QS(I) + QSP)
    47.     M mF F V                    ENDIF
    48.     M mF F V
    49.     M mF F V                    FSK(I,K,1) =  QAV(I,J,K,1) * QS(I)
    50.     M mF F V                    FSK(I,K,2) =  QAV(I,J,K,2) * QS(I) +
    51.     M mF F V              >                                 PAV(I,J,K) * SKX(I,J,K)
    52.     M mF F V                    FSK(I,K,3) =  QAV(I,J,K,3) * QS(I) +
    53.     M mF F V              >                                 PAV(I,J,K) * SKY(I,J,K)
    54.     M mF F V                    FSK(I,K,4) =  QAV(I,J,K,4) * QS(I) +
    55.     M mF F V              >                                 PAV(I,J,K) * SKZ(I,J,K)
    56.     M mF F V                    FSK(I,K,5) = (QAV(I,J,K,5) + PAV(I,J,K)) *
    57.     M mF F V              >                                                      QS(I)
```

Notice that Reveal doesn't use default shared, primarily to illustrate that it has handled all variables

Perftools-lite profiles

Original running on 8 nodes x 1 MPI/Node

```
Table 1:  Profile by Function (limited entries shown)
  Samp% |      Samp | Imb.  |  Imb.  | Group
        |           | Samp  | Samp%  |  Function=[MAX10]
        |           |       |        |   PE=HIDE
 100.0% | 29,633.0  |   --  |    --  | Total
|-------------------------------------------------
|  98.5% | 29,183.5 |    -- |     -- | USER
||------------------------------------------------
||  27.1% |  8,030.6 | 43.4  |  0.6%  | fluxj_
||  26.9% |  7,958.6 | 47.4  |  0.7%  | fluxk_
||  22.8% |  6,745.0 | 79.0  |  1.3%  | fluxi_
||   5.2% |  1,551.4 | 21.6  |  1.6%  | extrapk_
||   5.1% |  1,499.5 | 18.5  |  1.4%  | extrapi_
||   4.6% |  1,376.2 | 24.8  |  2.0%  | update_
||   4.2% |  1,258.9 | 24.1  |  2.1%  | extrapj_
||================================================
|   1.4% |    407.9 |   --  |    --  | MPI
|================================================
```

Threaded is 26 times faster on 44 threads. However, the MPI is only using one thread, lets run 44 MPI tasks on the node

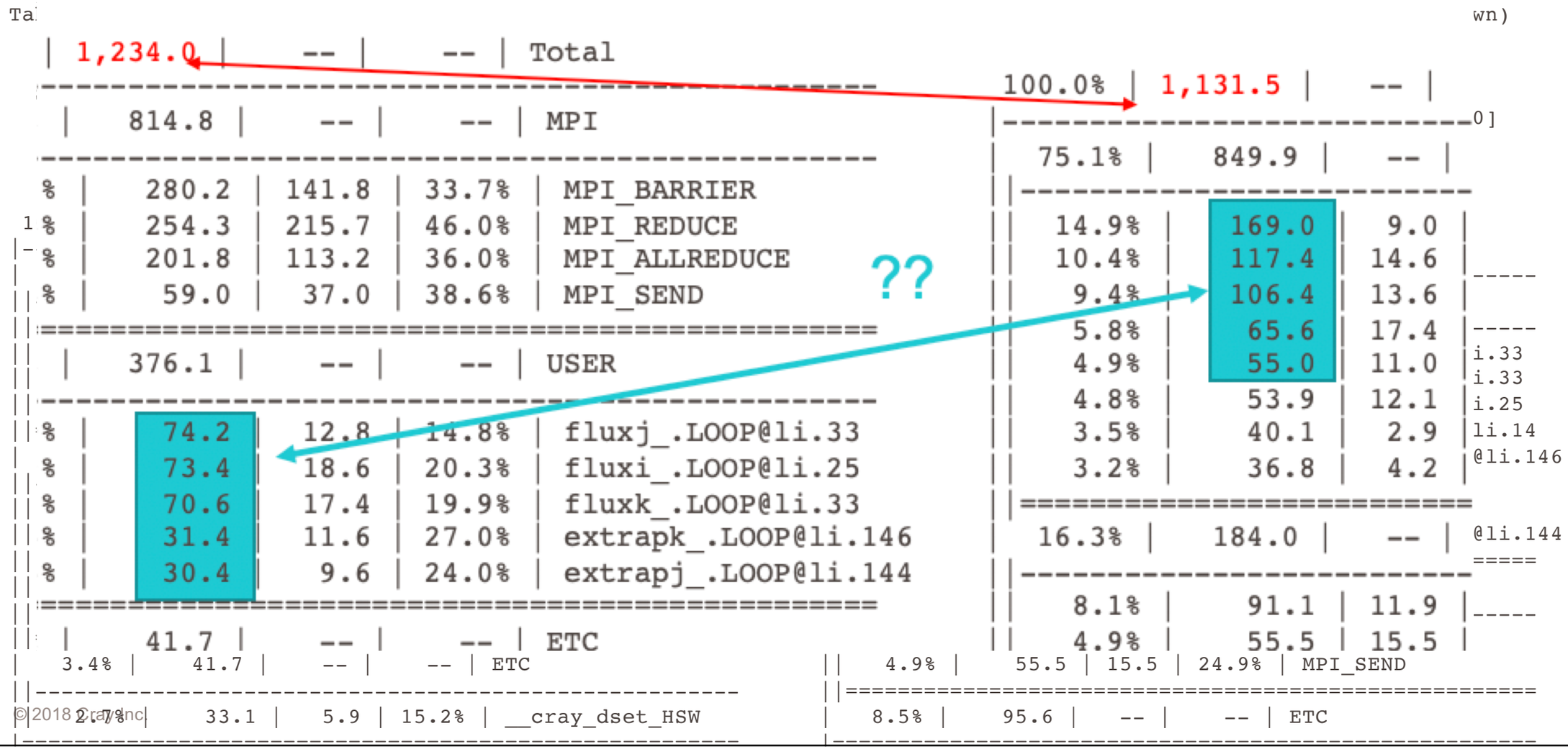
Threaded running on 8 nodes 1 MPIx44 threads /Node

```
  Samp% |      Samp | Imb.  |  Imb.  | Group
        |           | Samp  | Samp%  |  Function=[MAX10]
        |           |       |        |   PE=HIDE
        |           |       |        |    Thread=HIDE
 100.0% | 1,131.5   |   --  |    --  | Total
|-------------------------------------------------
|  75.1% |   849.9  |    -- |     -- | USER
||------------------------------------------------
||  14.9% |   169.0  |  9.0  |  5.8%  | fluxk_.LOOP@li.33
||  10.4% |   117.4  | 14.6  | 12.7%  | fluxj_.LOOP@li.33
||   9.4% |   106.4  | 13.6  | 13.0%  | fluxi_.LOOP@li.25
||   5.8% |    65.6  | 17.4  | 23.9%  | update_.LOOP@li.14
||   4.9% |    55.0  | 11.0  | 19.0%  | extrapk_.LOOP@li.146
||   4.8% |    53.9  | 12.1  | 21.0%  | mpicx_
||   3.5% |    40.1  |  2.9  |  7.6%  | tmstep_
||   3.2% |    36.8  |  4.2  | 11.8%  | extrapj_.LOOP@li.144
||================================================
|  16.3% |   184.0  |   --  |    --  | MPI
||------------------------------------------------
||   8.1% |    91.1  | 11.9  | 13.2%  | MPI_REDUCE
||   4.9% |    55.5  | 15.5  | 24.9%  | MPI_SEND
||================================================
|   8.5% |    95.6  |   --  |    --  | ETC
|-------------------------------------------------
```

Perftools-lite profiles

Original running on 8 nodes x 44 MPI

Threaded running on 8 nodes 1 MPIx44 threads/Node



Why are the OpenMP loops doing poorly?

Table 3: Memory Bandwidth by Numanode (limited entries shown)

Memory Traffic GBytes	Local Memory Traffic GBytes	Remote Memory Traffic GBytes	Thread Time	Memory Traffic GBytes / Sec	Memory Traffic / Nominal Peak	Numanode Node Id=[max3,min3] PE=HIDE Thread=HIDE
184.47	173.59	10.89	11.578777	15.93	20.7%	numanode.0
183.50	173.59	9.91	11.569322	15.86	20.7%	nid.63
182.61	172.40	10.21	11.578777	15.77	20.5%	nid.61
178.55	167.75	10.80	11.563156	15.44	20.1%	nid.71
178.10	168.14	9.96	11.562097	15.40	20.1%	nid.62
178.08	168.07	10.01	11.564512	15.40	20.1%	nid.68
178.01	167.20	10.82	11.572032	15.38	20.0%	nid.70
60.36	14.73	45.62	9.073119	6.65	8.7%	numanode.1
60.36	14.73	45.62	9.072693	6.65	8.7%	nid.63
59.88	14.33	45.55	9.071553	6.60	8.6%	nid.62
59.48	14.19	45.29	9.068044	6.56	8.5%	nid.68
58.78	13.70	45.08	9.069259	6.48	8.4%	nid.70
58.67	13.87	44.81	9.071591	6.47	8.4%	nid.69
58.53	13.86	44.67	9.067146	6.46	8.4%	nid.71

The threads on socket 0 have great local memory bandwidth because they are accessing most of their data on socket 0.

The threads on socket 1 have bad remote memory bandwidth because they are accessing most of their data off socket 0.

This is the NUMA traffic from the all-MPI run.

Table 3: Memory Bandwidth by Numanode (limited entries shown)

Memory Traffic GBytes	Local Memory Traffic GBytes	Remote Memory Traffic GBytes	Thread Time	Memory Traffic GBytes / Sec	Memory Traffic / Nominal Peak	Numanode Node Id=[max3,min3] PE=HIDE
172.95	171.48	1.48	19.755654	8.75	11.4%	numanode.0
172.77	171.48	1.30	19.414237	8.90	11.6%	nid.68
172.09	170.61	1.48	19.071340	9.02	11.7%	nid.63
171.20	169.93	1.27	17.631761	9.71	12.6%	nid.62
162.51	161.07	1.43	19.675857	8.26	10.8%	nid.71
162.28	160.82	1.46	19.730793	8.22	10.7%	nid.72
161.75	160.29	1.46	19.755654	8.19	10.7%	nid.70
168.69	166.81	1.89	19.781479	8.53	11.1%	numanode.1
168.69	166.81	1.89	19.454144	8.67	11.3%	nid.62
167.74	166.03	1.71	19.476164	8.61	11.2%	nid.63
166.66	164.88	1.78	19.225409	8.67	11.3%	nid.61
161.68	160.07	1.61	19.781479	8.17	10.6%	nid.71
161.60	159.99	1.62	19.642791	8.23	10.7%	nid.70
157.32	156.01	1.31	18.036118	8.72	11.4%	nid.72

Since each MPI task has data on the same socket that it is running on its local memory memory bandwidth is great

While the OpenMP is still running a little faster

- Why are each of the major computational routines running slower than the MPI version?
  - We are running 44 threads across two sockets within the node
    - When memory is initialized – in this case by the master thread, the variables will be allocated in the first socket's memory
    - Each socket can access its own memory faster than it can access the other nodes memory
    - Therefore the threads on second socket will be penalized if it has to access memory on the first socket.
    - Then we will have load imbalance between the OpenMP threads

Why is MPI getting better scaling than OpenMP on the node

- OpenMP run
  - setenv OMP_NUM_THREADS 44
  - aprun -n 8 -N 1 -d 44 ./xleslie3d_mpi > out8on8_44
- MPI run
  - setenv OMP_NUM_THREADS 1
  - aprun -n 352 -N 44 ./xleslie3d_mpi > all_mpi
- Improved OpenMP
  - setenv OMP_NUM_THREADS 22
  - aprun -n 8 -N 2 –S 1 -d 22 ./xleslie3d_mpi > out8on8_44

Running across two sockets will incur NUMA issues

Running with a MPI task on each socket and 22 threads/MPI task

Perftools-lite profiles

Original running on 8 nodes x 44 MPI

Threaded running on 8 nodes 2 MPIx22 threads/Node

Ahh – Much Better

PE=HIDE

Tab

0%	1,234.0	--	--	Total
.0%	814.8	--	--	MPI
2.7%	280.2	141.8	33.7%	MPI_BARRIER
0.6%	254.3	215.7	46.0%	MPI_REDUCE
6.4%	201.8	113.2	36.0%	MPI_ALLREDUCE
4.8%	59.0	37.0	38.6%	MPI_SEND
.5%	376.1	--	--	USER
6.0%	74.2	12.8	14.8%	fluxj_.LOOP@li.33
5.9%	73.4	18.6	20.3%	fluxi_.LOOP@li.25
5.7%	70.6	17.4	19.9%	fluxk_.LOOP@li.33
2.5%	31.4	11.6	27.0%	extrapk_.LOOP@li.146
2.5%	30.4	9.6	24.0%	extrapj_.LOOP@li.144

2.5%	30.4	9.6	24.0%	extrapj_.LOOP@li.144
3.4%	41.7	--	--	ETC
2.7%	33.1	5.9	15.2%	__cray_dset_HSW

100.0%	843.8	--	--	T
55.0%	463.9	--	--	
9.9%	83.1	9.9	11.3%	
9.2%	77.6	8.4	10.5%	
8.7%	73.3	14.7	17.8%	
3.6%	30.1	8.9	24.3%	
3.5%	29.8	10.2	27.3%	
3.4%	28.4	6.6	20.0%	
37.4%	315.4	--	--	
19.4%	164.0	51.0	25.3%	
9.4%	79.1	36.9	33.9%	
6.4%	54.1	27.9	36.3%	

7.5%	63.2	--	--	ETC
2.9%	24.2	0.8	3.5%	__cray_dset_HSW

Let's look at perftools-lite-hbm

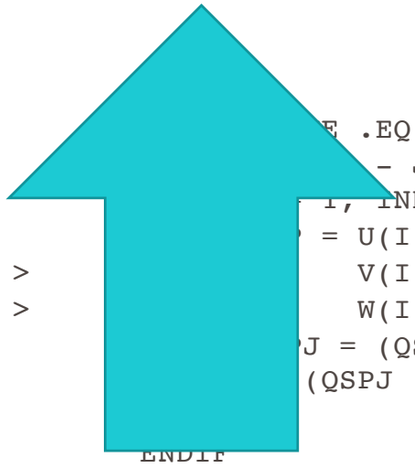
```
Table 5:  Profile by Group, Function, and Line (limited entries shown)

||||-------------------------------------------------------------------------
4|||   4.2% |  2.5 |  1.5 | 42.9% |   246,290,604,776,946 |  11,331,973,206 | line.36
4|||   7.8% |  4.6 |  5.4 | 61.4% |   387,028,093,089,632 |  18,250,631,160 | line.72
4|||   8.0% |  4.8 |  4.2 | 54.0% |   316,659,349,107,561 |  16,880,190,381 | line.81
||||=========================================================================

 ||
 ||  23.5% | 14.0 |   -- |    -- | 1,231,453,023,644,5    56,564,956,788 | fluxj_
 3|        |      |      |        |                        |                |  fluxj.f
 ||||-------------------------------------------------------------------------
 4|||   4.2% |  2.5 |  1.5 | 42.9% |   246,290,604,776,946 |  11,331,973,206 | line.36
 4|||   7.8% |  4.6 |  5.4 | 61.4% |   387,028,093,089,632 |  18,250,631,160 | line.72
 4|||   8.0% |  4.8 |  4.2 | 54.0% |   316,659,349,107,561 |  16,880,190,381 | line.81
 ||||=========================================================================
 ||  23.3% | 13.9 |   -- |    -- | 1,618,481,116,517,358 |  46,077,159,986 | fluxi_
 3|        |      |      |        |                        |                |  fluxi.f
 ||||-------------------------------------------------------------------------
 4|||   5.7% |  3.4 |  1.6 | 37.1% |   316,659,348,989,901 |   9,236,821,683 | line.29
 4|||   1.5% |  0.9 |  2.1 | 81.0% |    70,368,744,186,054 |   5,096,471,788 | line.41
 4|||   1.1% |  0.6 |  1.4 | 78.6% |    70,368,744,181,663 |   2,885,621,509 | line.42
 4|||   1.7% |  1.0 |  1.0 | 57.1% |   105,553,116,300,240 |   5,639,566,321 | line.48
 4|||   7.8% |  4.6 |  3.4 | 48.2% |   668,503,069,752,688 |  13,084,700,740 | line.61
 4|||   4.8% |  2.9 |  1.1 | 32.1% |   316,659,348,925,684 |   7,922,852,884 | line.68
```

Let's look at perftools-lite-hbm

```
    28.                          ! Directive inserted by Cray Reveal.  May be incomplete.
    29.    M--------------------< !$OMP  parallel do default(none)
51.  + M mF F fF-----------<>              FSJ(1:IND,J,1) =  QAV(1:IND,J,K,1) * QS(1:IND)
52.  + M mF F fF-----------<>              FSJ(1:IND,J,2) =  QAV(1:IND,J,K,2) * QS(1:IND) +
53.    M mF F                      >                          PAV(1:IND,J,K) * SJX(1:IND,J,K)
54.  + M mF F fF-----------<>              FSJ(1:IND,J,3) =  QAV(1:IND,J,K,3) * QS(1:IND) +
55.    M mF F                      >                          PAV(1:IND,J,K) * SJY(1:IND,J,K)
```



```
    39.    M mF F
    40.    M mF F                                    E .EQ. 2) THEN
    41.    M mF F                                    - JADD
    42.    M mF F D-------------<                    1, IND
    43.    M mF F D                                  = U(I,L,K) * SJX(I,J,K) +
    44.    M mF F D                    >               V(I,L,K) * SJY(I,J,K) +
    45.    M mF F D                    >               W(I,L,K) * SJZ(I,J,K)
    46.    M mF F D                                  J = (QSP - QS(I)) * DBLE(1 - 2 *
    47.    M mF F D                                  (QSPJ .GT. 0.0D+00) QS(I) = 0.5D+
    48.    M mF F D-------------->
    49.    M mF F                                    ENDIF
    50.    M mF F
    51.  + M mF F fF-----------<>              FSJ(1:IND,J,1) =  QAV(1:IND,J,K,1) * QS(1:I
    52.  + M mF F fF-----------<>              FSJ(1:IND,J,2) =  QAV(1:IND,J,K,2) * QS(1:I
    53.    M mF F                      >                          PAV(1:IND,J,K) * SJX(
    54.  + M mF F fF-----------<>              FSJ(1:IND,J,3) =  QAV(1:IND,J,K,3) * QS(1:IND) +
    55.    M mF F                      >                          PAV(1:IND,J,K) * SJY(1:IND,J,K)
```

Array syntax is very poor for cache based systems.

The compiler is even fusing 36-38 with 51-55

Rewritten with loops

```
28.   + F------------------<        DO K = 1, KCMAX
29.   + F F----------------<           DO J = 0, JCMAX
30.     F F V--------------<             DO I = 1, IND
31.     F F V                             QS(I) = UAV(I,J,K) * SJX(I,J,K) +
32.     F F V                   >                 VAV(I,J,K) * SJY(I,J,K) +
33.     F F V                   >                 WAV(I,J,K) * SJZ(I,J,K)
34.     F F V
35.     F F V                             IF (NSCHEME .EQ. 2) THEN
36.     F F V                                L = J + 1 - JADD
37.     F F V
38.     F F V                                QSP = U(I,L,K) * SJX(I,J,K) +
39.     F F V                   >                  V(I,L,K) * SJY(I,J,K) +
40.     F F V                   >                  W(I,L,K) * SJZ(I,J,K)
41.     F F V                                QSPJ = (QSP - QS(I)) * DBLE(1 - 2 * JADD)
42.     F F V                                IF (QSPJ .GT. 0.0D+00) QS(I) = 0.5D+00 * (QS(I) + QSP)
43.     F F V
44.     F F V                             ENDIF
45.     F F V
46.     F F V                           FSJ(I,J,1) =  QAV(I,J,K,1) * QS(I)
47.     F F V                           FSJ(I,J,2) =  QAV(I,J,K,2) * QS(I) +
48.     F F V                   >                                PAV(I,J,K) * SJX(I,J,K)
49.     F F V                           FSJ(I,J,3) =  QAV(I,J,K,3) * QS(I) +
```

Let's look at perftools-lite-hbm

```
73.     M mF
74.   + M mF ib--------------<         DO J = 1, JCMAX
75.   + M mF ib ib------------<            DO L = 1, 5
76.     M mF ib ib Vbr2-----<>                DQ(1:IND,J,K,L) = DQ(1:IND,J,K,L) -
77.     M mF ib ib                  >             DTV(1:IND,J,K) * (FSJ(1:IND,J,L) - FSJ(1:IND,J-1,L))
78.     M mF ib ib------------>               ENDDO
79.     M mF ib
80.     M mF ib                               IF (ISGSK .EQ. 1) THEN
81.     M mF ib                                  DQ(1:IND,J,K,7) = DQ(1:IND,J,K,7) -
82.     M mF ib                     >             DTV(1:IND,J,K) * (FSJ(1:IND,J,7) - FSJ(1:IND,J-1,7))
83.     M mF ib                               ENDIF
84.     M mF ib
85.     M mF ib                               IF ( ICHEM .GT. 0 ) THEN
86.     M mF ib D-------------<                  DO L = 8, 7 + NSPECI
87.     M mF ib D                                  DQ(1:IND,J,K,L) = DQ(1:IND,J,K,L) -
88.     M mF ib D                   >                DTV(1:IND,J,K) * (FSJ(1:IND,J,L) - FSJ(1:IND,J-1,L))
89.     M mF ib D------------>                  ENDDO
90.     M mF ib                                 ENDIF
91.     M mF ib--------------->              ENDDO
92.     M mF----------------->>           ENDDO
```

Be careful of compiler's' automatic blocking

Rewritten with loops and directives

```
70.     F                    !dir$ noblocking
71.   + F ir2--------------<         DO J = 1, JCMAX
72.     F ir2                !dir$ noblocking
73.     F ir2 iVr2---------<            DO I = 1, IND
74.     F ir2 iVr2           !dir$ noblocking
75.   + F ir2 iVr2 ir2-----<              DO L = 1, 5
76.     F ir2 iVr2 ir2                       DQ(I,J,K,L) = DQ(I,J,K,L) -
77.     F ir2 iVr2 ir2             >              DTV(I,J,K) * (FSJ(I,J,L) - FSJ(I,J-1,L))
78.     F ir2 iVr2 ir2----->                ENDDO
79.     F ir2 iVr2
80.     F ir2 iVr2                          IF (ISGSK .EQ. 1) THEN
81.     F ir2 iVr2                             DQ(I,J,K,7) = DQ(I,J,K,7) -
82.     F ir2 iVr2                 >              DTV(I,J,K) * (FSJ(I,J,7) - FSJ(I,J-1,7))
83.     F ir2 iVr2                          ENDIF
84.     F ir2 iVr2
85.     F ir2 iVr2                          IF ( ICHEM .GT. 0 ) THEN
86.     F ir2 iVr2 D-------<                   DO L = 8, 7 + NSPECI
87.     F ir2 iVr2 D                              DQ(I,J,K,L) = DQ(I,J,K,L) -
88.     F ir2 iVr2 D               >                DTV(I,J,K) * (FSJ(I,J,L) - FSJ(I,J-1,L))
89.     F ir2 iVr2 D------->                   ENDDO
90.     F ir2 iVr2                          ENDIF
91.     F ir2 iVr2--------->              ENDDO
92.     F ir2-------------->            ENDDO
93.     F------------------>          ENDDO
```

Perftools-lite profiles

After removing array syntax

Table 1: Profile by Function (limited entries shown)

```
100.0% | 803.9 |   -- |    -- | Total
|-----------------------------------------------
|  54.0% | 433.8 |   -- |    -- | USER
||----------------------------------------------
||   9.7% |  78.0 |  6.0 |  7.6% | fluxk_.LOOP@li.32
||   8.5% |  68.3 |  7.7 | 10.8% | fluxj_.LOOP@li.32
||   8.1% |  65.1 |  5.9 |  8.8% | fluxi_.LOOP@li.25
||   3.5% |  28.4 |  3.6 | 12.1% | extrapk_.LOOP@li.150
||   3.3% |  26.8 | 12.2 | 33.5% | mpicx_
||   3.3% |  26.6 |  2.4 |  9.0% | update_.LOOP@li.14
||===============================================
|  37.7% | 302.8 |   -- |    -- | MPI
||----------------------------------------------
||  22.0% | 176.8 | 56.2 | 25.8% | MPI_REDUCE
||  10.2% |  81.7 | 46.3 | 38.6% | MPI_ALLREDUCE
||   3.9% |  31.2 | 14.8 | 34.2% | MPI_SEND
||===============================================
|   8.2% |  66.0 |   -- |    -- | ETC
||----------------------------------------------
||   3.1% |  25.3 |  1.7 |  6.7% | __cray_dset_HSW
```

Table 1: Profile by Function (limited entries shown)

```
Samp% |  Samp | Imb. |  Imb. | Group
100.0% | 843.8 |   -- |    -- | Total
|-----------------------------------------
|  55.0% | 463.9 |   -- |    -- | USER
||----------------------------------------
||   9.9% |  83.1 |  9.9 | 11.3% | fluxk
||   9.2% |  77.6 |  8.4 | 10.5% | fluxj
||   8.7% |  73.3 | 14.7 | 17.8% | fluxi
||   3.6% |  30.1 |  8.9 | 24.3% | extra
||   3.5% |  29.8 | 10.2 | 27.3% | mpicx
||   3.4% |  28.4 |  6.6 | 20.0% | updat
||========================================
|  37.4% | 315.4 |   -- |    -- | MPI
||----------------------------------------
||  19.4% | 164.0 | 51.0 | 25.3% | MPI_REDUCE
||   9.4% |  79.1 | 36.9 | 33.9% | MPI_ALLREDUCE
||   6.4% |  54.1 | 27.9 | 36.3% | MPI_SEND
||========================================
|   7.5% |  63.2 |   -- |    -- | ETC
||----------------------------------------
||   2.9% |  24.2 |  0.8 |  3.5% | __cray_dset_HSW
|========================================
```

So lets add OpenMP Accelerator directives

```
#ifdef OMP_TARGET
!$omp target teams distribute
!$omp&    private(fsi,i,j,k,l,qs,qsp,qspi)
#else
! Directive inserted by Cray Reveal.  May be incomplete.
!$OMP  parallel do default(none)
!$OMP&   private (fsi,i,j,k,l,qs,qsp,qspi)
!$OMP&   shared  (dq,dtv,iadd,icmax,jcmax,kcmax,pav,qav,six,siy,siz,u,
!$OMP&            uav,v,vav,w,wav)
#endif
      DO K = 3, KCMAX, ICMAX
            QS(I) = UAV(I,J,K) * SIX(I,J,K) +
     >                VAV(I,J,K) * SIY(I,J,K) +
     >                WAV(I,J,K) * SIZ(I,J,K)


            IF ( NSCHEME .EQ. 2 ) THEN
                  L = I + 1 - IADD
                  QSP = U(L,J,K) * SIX(I,J,K) +
     >                  V(L,J,K) * SIY(I,J,K) +
     >                  W(L,J,K) * SIZ(I,J,K)
                  QSPI = (QSP - QS(I)) * DBLE(1 - 2 * IADD)
                  IF ( QSPI .GT. 0.0D0 ) QS(I) = 0.5D0 * (QS(I) + QSP)
            ENDIF
```

Only need to worry about private variables

Don’t worry about data movement yet

Reveal put these directives in

So lets add OpenMP Accelerator directives

```
21.  + G----------------< !$omp target teams distribute
22.    G                 !$omp&    private(fsi,i,j,k,l,qs,qsp,qspi)
23.    G                 #else
24.    D                 ! Directive inserted by Cray Reveal.  May be incomplete.
25.    D                 !$OMP  parallel do default(none)
26.    D                 !$OMP&   private (fsi,i,j,k,l,qs,qsp,qspi)
27.    D                 !$OMP&   shared  (dq,dtv,iadd,icmax,jcmax,kcmax,pav,qav,six,siy,siz,u,
28.    D                 !$OMP&            uav,v,vav,w,wav)
29.    G                 #endif
30.  + G gF-------------<       DO K = 1, KCMAX
31.  + G gF F-----------<          DO J = 1, JCMAX
32.    G gF F
33.  + G gF F fgF------<>             QS(0:ICMAX) = UAV(0:ICMAX,J,K) * SIX(0:ICMAX,J,K) +
34.    G gF F                >                    VAV(0:ICMAX,J,K) * SIY(0:ICMAX,J,K) +
35.    G gF F                >                    WAV(0:ICMAX,J,K) * SIZ(0:ICMAX,J,K)
36.    G gF F
37.    G gF F                             IF ( NSCHEME .EQ. 2 ) THEN
38.    G gF F D---------<                    DO I = 0, ICMAX
39.    G gF F D                                 L = I + 1 - IADD
40.    G gF F D                                 QSP = U(L,J,K) * SIX(I,J,K) +
41.    G gF F D              >                        V(L,J,K) * SIY(I,J,K) +
42.    G gF F D              >                        W(L,J,K) * SIZ(I,J,K)
43.    G gF F D                                 QSPI = (QSP - QS(I)) * DBLE(1 - 2 * IADD)
44.    G gF F D                                 IF ( QSPI .GT. 0.0D0 ) QS(I) = 0.5D0 * (QS(I) + QSP)
45.    G gF F D--------->                    ENDDO
46.    G gF F                             ENDIF
```

So lets add Accelerator directives

Let the compiler figure out data movement

```
ftn-6418 ftn: ACCEL FLUXI, File = fluxi.f, Line = 21
  If not already present: allocate memory and copy whole array "siy" to accelerator, free at line 93 (acc_copyin).

ftn-6418 ftn: ACCEL FLUXI, File = fluxi.f, Line = 21
  If not already present: allocate memory and copy whole array "vav" to accelerator, free at line 93 (acc_copyin).

ftn-6418 ftn: ACCEL FLUXI, File = fluxi.f, Line = 21
  If not already present: allocate memory and copy whole array "six" to accelerator, free at line 93 (acc_copyin).

ftn-6418 ftn: ACCEL FLUXI, File = fluxi.f, Line = 21
  If not already present: allocate memory and copy whole array "uav" to accelerator, free at line 93 (acc_copyin).

ftn-6418 ftn: ACCEL FLUXI, File = fluxi.f, Line = 21
  If not already present: allocate memory and copy whole array "siz" to accelerator, free at line 93 (acc_copyin).

ftn-6418 ftn: ACCEL FLUXI, File = fluxi.f, Line = 21
  If not already present: allocate memory and copy whole array "wav" to accelerator, free at line 93 (acc_copyin).

ftn-6418 ftn: ACCEL FLUXI, File = fluxi.f, Line = 21
  If not already present: allocate memory and copy whole array "qav" to accelerator, free at line 93 (acc_copyin).
```

Approach for turning OpenMP threading into OpenMP Accelerator Directives

- Will also use perftools to investigate accelerator performance
  - Module load perftools instead of perftools-lite
    - Perftools-lite-gpu doesn't show much right now
  - After building application pat_build –u –g mpi <executable>
  - Run <executable+pat>
  - pat_report < directory created when running <executable+pat>>

Profile from first cut at OpenMP Offload

```
Table 1:  Profile by Function Group and Function

  Time% |        Time |     Imb. |  Imb. |    Calls | Group
        |             |     Time | Time% |          |  Function
100.0% | 192.065111 |       -- |    -- | 22,492.0 | Total
|-------------------------------------------------------------------------
|  96.3% | 184.972019 |       -- |    -- |  9,400.0 | OACC
||------------------------------------------------------------------------
||  17.1% |  32.847375 | 0.018724 |  0.1% |    200.0 | fluxi_.ACC_COPY@li.29
||  15.8% |  30.296096 | 0.020366 |  0.1% |    200.0 | fluxk_.ACC_COPY@li.24
||  15.8% |  30.291321 | 0.018862 |  0.1% |    200.0 | fluxj_.ACC_COPY@li.24
||  13.5% |  25.842807 | 0.003061 |  0.0% |    200.0 | fluxi_.ACC_COPY@li.266
||  12.4% |  23.890719 | 0.003862 |  0.0% |    200.0 | fluxj_.ACC_COPY@li.109
||  12.4% |  23.889958 | 0.001421 |  0.0% |    200.0 | fluxk_.ACC_COPY@li.106
||   4.1% |   7.804356 | 0.015985 |  0.3% |    200.0 | update_.ACC_COPY@li.10
||   1.0% |   1.962536 | 0.000358 |  0.0% |    200.0 | fluxi_.ACC_SYNC_WAIT@li.265
||=========================================================================
|   2.9% |   5.591116 |       -- |    -- |  6,546.0 | USER
||-------------------------------------------------------------------------
```

Copies to and from the GPU

Waiting for GPU kernel to finish

Approach for turning OpenMP threading into OpenMP Accelerator Directives

- First convert all OpenMP high level loops into OpenMP Accelerator Directives
- Next introduce DATA regions up the call tree
    - Insert appropriate data updates and move more loops to the accelerator

Perftools-lite loops – Run on 8 nodes–8 MPI tasks

Can we introduce DATA regions here?

```
Table 1:  Function Calltree View (limited entries shown)
  Time% |       Time |       Calls | Calltree
        |            |             |  PE=HIDE
 100.0% | 331.356157 |          -- | Total
|-----------------------------------------------------------
| 100.0% | 331.356117 |         2.0 | les3d_
|  99.3% | 329.201866 |          -- |  les3d_.LOOP.3.li.216
3  98.7% | 327.029239 |          -- |   les3d_.LOOP.4.li.272
||||-----------------------------------------------------
4|||  31.6% | 104.588754 |     1,000.0 | fluxk_
|||||-----------------------------------------------------
5||||  20.2% |  66.813949 |          -- | fluxk_.LOOP.1.li.28
6||||        |            |             |  fluxk_.LOOP.2.li.29
7||||  20.2% |  66.813949 | 9,312,000.0 |   visck_
5||||   6.4% |  21.068680 |     1,000.0 | fluxk_(exclusive)
5||||   5.0% |  16.706125 |     1,000.0 | extrapk_
|||||=====================================================
4|||  29.2% |  96.783424 |     1,000.0 | fluxi_
|||||-----------------------------------------------------
5||||  16.9% |  55.929620 |          -- | fluxi_.LOOP.1.li.21
6||||        |            |             |  fluxi_.LOOP.2.li.22
7||||  16.9% |  55.929620 | 9,216,000.0 |   visci_
5||||   6.8% |  22.465390 |     1,000.0 | extrapi_
||||||----------------------------------------------------
6|||||   3.4% |  11.399343 |     1,000.0 | extrapi_(exclusive)
6|||||   3.3% |  11.066047 |          -- | extrapi_.LOOP.1.li.128
7|||||       |            |             |  extrapi_.LOOP.2.li.129
8|||||   3.3% |  11.066047 | 9,801,000.0 |   exi4_
||||||=====================================================
5||||   5.5% |  18.388414 |     1,000.0 | fluxi_(exclusive)
|||||=====================================================
4|||  28.4% |  93.988073 |     1,000.0 | fluxj_
|||||-----------------------------------------------------
5||||  18.3% |  60.687484 |          -- | fluxj_.LOOP.1.li.28
6||||        |            |             |  fluxj_.LOOP.2.li.29
7||||  18.3% |  60.687484 | 9,312,000.0 |   viscj_
5||||   5.9% |  19.520634 |     1,000.0 | fluxj_(exclusive)
5||||   4.2% |  13.779955 |     1,000.0 | extrapj_
|||||=====================================================
4|||   5.3% |  17.668610 |     1,000.0 | parallel_
|||||-----------------------------------------------------
5||||   4.0% |  13.109379 |          -- | parallel_.LOOP.1.li.16
6||||   4.0% |  13.109379 |     5,000.0 |  mpicx_
5||||   1.4% |   4.543585 |     4,000.0 | ghost_
|||||=====================================================
```

So we insert OpenMP 4.5 target data region

```
216.  +              !$omp target data map(tofrom:P,Q,SIY,VAV,SIX,UAV,SIZ,WAV,QAV,PAV,U,V,
217.                 !$omp&        W,T,Y,W,T11,T21,EKAV,EK,DS,DS1,T31,TAV,T12,T22,T32,T13,
218.                 !$omp&        T23,T33,HF,DTV,DQ)
220.  + 1----------<       DO WHILE ( NADV .LE. NEND .AND. TAU .LT. 35.0D+00 )
221.    1
222.    1                    IF ( MOD ( NADV, ITIME ) .EQ. 0 .OR. NADV .EQ. NSTART )
223.  + 1                 >                              CALL TMSTEP ( TMAX, RMACH )
224.    1
225.    1                    TIME = TIME + DT
226.    1
227.  + 1                    CALL ANALYSIS ( TAU, DELM )
228.    1
229.    1                    IF ( IAM .EQ. 0 .AND. MOD ( NADV, ITIME ) .EQ. 0 ) THEN
230.    1                       WRITE(6,1000) NADV, DT, TIME, TAU, DELM
231.    1                       WRITE(50,'(2(F10.5,1X))') TAU, DELM
232.    1                    ENDIF
233.    1              1000  FORMAT(' NADV = ', I6,
234.    1                   >        ' DT   = ', E10.4,
235.    1                   >        ' TIME = ', F8.5,
236.    1                   >        ' TAU  = ', F8.4,
237.    1                   >        ' DELM = ', F8.4)
238.    1
239.    1
240.    1                    IF ( IDYN .GT. 0 ) THEN
241.  + 1                       CALL EJECT ( 'LDKM, PLEASE RECOMPILE WITH -DLDKM!' )
242.    1                    ENDIF
243.    1
244.    1                    IADD = MOD ( NADV, 2 )
```

But then you have added a ton of work to do

- You now have two copies of the data that has been moved to the accelerator
  - Every place data is used that resides on the accelerator and on the host, the user is responsible for moving data back to host when computation requires an updated copy of the data
  - I know about unified memory; however, often times is will not do as good a job as the user and we do not have it right now
- Put as much computation on the accelerator as possible
- In this case halo exchanges require some treatment

Within the Data region

```
316.     1 2
317.     1 2                       IF ( ISTART .EQ. 1 .AND. INFLOW .EQ. 1 ) THEN
318.     1 2                          I = 0
319.     1 2           #ifdef GPU
320.     1 2           !$omp target teams distribute
321.     1 2           !$omp&           map(to:bound)
322.     1 2           !$omp&            map(from:q,t)
323.     1 2           !$omp&            private(l)
324.     1 2           #else
325.     D             !$OMP PARALLEL DO PRIVATE(L)
326.     1 2           #endif
327.     1 2 D------<                 DO K = 1, KCMAX
328.     1 2 D 4----<                    DO J = 1, JCMAX
329.     1 2 D 4                            Q(I,J,K,1,M) = BOUND(J,K,1)
330.     1 2 D 4                            Q(I,J,K,2,M) = BOUND(J,K,1) * BOUND(J,K,2)
331.     1 2 D 4                            Q(I,J,K,3,M) = BOUND(J,K,1) * BOUND(J,K,3)
332.     1 2 D 4                            Q(I,J,K,4,M) = BOUND(J,K,1) * BOUND(J,K,4)
333.     1 2 D 4                            T(I,J,K)     = BOUND(J,K,5)
334.     1 2 D 4                            IF ( ICHEM .GT. 0 ) THEN
335.     1 2 D 4 5--<                          DO NS = 1, NSPECI
336.     1 2 D 4 5                                L = 7 + NS
337.     1 2 D 4 5                                Q(I,J,K,L,M) = BOUND(J,K,1) * BOUND(J,K,L)
338.     1 2 D 4 5-->                          ENDDO
339.     1 2 D 4                            ENDIF
340.     1 2 D 4                            IF ( ISGSK .EQ. 1 ) THEN
341.     1 2 D 4                               Q(I,J,K,7,M) = BOUND(J,K,1) * BOUND(J,K,7)
342.     1 2 D 4                            ENDIF
343.     1 2 D 4---->                    ENDDO
344.     1 2 D------>                 ENDDO
345.     1 2                       ENDIF
346.     1 2
```

Any computation within the data block must either be put on the accelerator or the data read has to be updated on the host.

This loop we move to the Accelerator

Halo exchange within the Data region

```
346.     1 2
347.     1 2           ! Exchange boundary information
348.     1 2
349.     1 2           #ifdef GPU
350.     1 2           !$omp target update from(q,hf)
351.     1 2           #endif
352.     1 2                     IF ( NSCHEME .EQ. 2 ) THEN
353.     1 2           !             CALL PARALLEL(2000 + N, 1)
354.   + 1 2                       CALL PARALLEL(2000 + N)
355.     1 2                     ELSE
356.     1 2           !             CALL PARALLEL(2000 + N, 2)
357.   + 1 2                       CALL PARALLEL(2000 + N)
358.     1 2                     ENDIF
359.     1 2           #ifdef GPU
360.     1 2           !$omp target update to(q,u,v,w)
361.     1 2           #endif
```

Perftools loaded – pat_build –u –g mpi <exe>

```
Table 1:  Profile by Function Group and Function
  Time% |      Time |     Imb. |  Imb. |    Calls | Group
        |           |     Time | Time% |          |  Function
        |           |          |       |          |   PE=HIDE
        |           |          |       |          |    Thread=HIDE
 100.0% | 48.808788 |       -- |    -- | 20,933.0 | Total
|-------------------------------------------------------------------------
|  85.5% | 41.721597 |       -- |    -- | 11,003.0 | OACC
||------------------------------------------------------------------------
||  27.7% | 13.512695 | 0.040378 |  0.6% |    200.0 | les3d_.ACC_COPY@li.355
||  20.3% |  9.926572 | 0.001944 |  0.0% |    200.0 | les3d_.ACC_COPY@li.345
||   7.2% |  3.491549 | 0.003118 |  0.2% |    200.0 | fluxi_.ACC_SYNC_WAIT@li.92
||   6.9% |  3.380262 | 0.003574 |  0.2% |    200.0 | fluxi_.ACC_SYNC_WAIT@li.108
```

```
||  27.7% | 13.512695 | 0.040378 |  0.6% |    200.0 | les3d_.ACC_COPY@li.355
||  20.3% |  9.926572 | 0.001944 |  0.0% |    200.0 | les3d_.ACC_COPY@li.345
||   4.3% |  2.099495 | 0.006041 |  0.6% |    200.0 | fluxj_.ACC_COPY@li.32
||   4.3% |  2.089182 | 0.006879 |  0.7% |    200.0 | fluxk_.ACC_COPY@li.31
||   1.5% |  0.718938 | 0.010417 |  2.9% |      1.0 | les3d_.ACC_COPY@li.216
||   1.2% |  0.567096 | 0.008023 |  2.8% |      1.0 | les3d_.ACC_COPY@li.415
```

```
||   1.0% |  0.471803 | 0.287358 | 75.7% |      1.0 | flowio_
||=========================================================================
|   1.7% |  0.845256 |       -- |    -- |  3,261.0 | MPI
||-------------------------------------------------------------------------
||   1.2% |  0.563471 | 0.175119 | 47.4% |      2.0 | MPI_REDUCE
|=========================================================================
```

ACC_COPY is data movement to and from the accelerator

Perftools loaded – pat_build –u –g mpi <exe>

```
Table 1:  Profile by Function Group and Function
  Time% |      Time |     Imb. |  Imb. |    Calls | Group
        |           |     Time | Time% |          |  Function
        |           |          |       |          |   PE=HIDE
        |           |          |       |          |    Thread=HIDE
 100.0% | 48.808788 |       -- |    -- | 20,933.0 | Total
||    7.2% |  3.491549 | 0.003118 |  0.2% |    200.0 | fluxi_.ACC_SYNC_WAIT@li.92
||    6.9% |  3.380262 | 0.003574 |  0.2% |    200.0 | fluxj_.ACC_SYNC_WAIT@li.108
||    6.8% |  3.340281 | 0.017049 |  1.0% |    200.0 | fluxk_.ACC_SYNC_WAIT@li.105

||    1.7% |  0.835638 | 0.000934 |  0.2% |    200.0 | extrapj_.ACC_SYNC_WAIT@li.240
||    1.5% |  0.748967 | 0.007268 |  1.9% |    200.0 | extrapk_.ACC_SYNC_WAIT@li.238
```

ACC_SYNC_WAIT is waiting for a kernel to finish

```
||    1.6% |  0.765046 | 0.011128 |  2.9% |      1.0 | setiv_
||    1.2% |  0.595023 | 0.000736 |  0.2% |  1,010.0 | mpicx_
||    1.0% |  0.500016 | 0.059047 | 21.1% |    202.0 | parallel_
||    1.0% |  0.471803 | 0.287358 | 75.7% |      1.0 | flowio_
||=============================================================================
|   1.7% |  0.845256 |       -- |    -- |  3,261.0 | MPI
||-----------------------------------------------------------------------------
||    1.2% |  0.563471 | 0.175119 | 47.4% |      2.0 | MPI_REDUCE
|=============================================================================
```

47.7% of the time is in updates for halo exchange

```
343.     1 2           ! Exchange boundary information
344.     1 2           #ifdef OMP_TARGET
345.     1 2           !$omp target update from(q,hf)
346.     1 2           #endif
347.     1 2                     IF ( NSCHEME .EQ. 2 ) THEN
348.     1 2           !             CALL PARALLEL(2000 + N, 1)
349.   + 1 2                        CALL PARALLEL(2000 + N)
350.     1 2                     ELSE
351.     1 2           !             CALL PARALLEL(2000 + N, 2)
352.   + 1 2                        CALL PARALLEL(2000 + N)
353.     1 2                     ENDIF
354.     1 2           #ifdef OMP_TARGET
355.     1 2           !$omp target update to(q,hf)
356.     1 2           #endif
```

So what is going on within PARALLEL

From our Call Tree --- pat_report –Oct –T.

```
3||   3.3% |  1.589344 |   200.0 | parallel_
||||-------------------------------------------------------------------
4|||   1.5% |  0.728695 | 1,000.0 | mpicx_
|||||-----------------------------------------------------------------
5||||   1.2% |  0.589571 | 1,000.0 | mpicx_(exclusive)
5||||   0.3% |  0.135674 | 1,000.0 | MPI_SEND
5||||   0.0% |  0.002217 | 1,000.0 | MPI_IRECV
5||||   0.0% |  0.001233 | 1,000.0 | MPI_WAIT
```

Down into PARALLEL and MPICX

```
      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')
       END IF
```

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--------->                DO I = 1-NLEVELS, ICMAX+NLEVELS
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

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

Two times faster

```
||  13.5% |  3.491808 | 0.000623 |  0.0% |    200.0 |
fluxi_.ACC_SYNC_WAIT@li.92
||  13.1% |  3.378351 | 0.003587 |  0.2% |    200.0 |
fluxj_.ACC_SYNC_WAIT@li.108
||  12.9% |  3.338869 | 0.016283 |  1.0% |    200.0 |
fluxk_.ACC_SYNC_WAIT@li.105

||   3.2% |  0.835128 | 0.000431 |  0.1% |    200.0 |
extrapj_.ACC_SYNC_WAIT@li.240
||   2.9% |  0.746907 | 0.005521 |  1.5% |    200.0 |
extrapk_.ACC_SYNC_WAIT@li.238

||   1.7% |  0.439470 | 0.000434 |  0.2% |    200.0 |
update_.ACC_SYNC_WAIT@li.45
||   1.2% |  0.315081 | 0.000720 |  0.5% |    200.0 |
extrapi_.ACC_SYNC_WAIT@li.172
```

Now most of the time is spent in kernel execution. Next step would be to investigate the performance of the top kernels to see if they can be improved

Two times faster

```
Table 1:  Profile by Function Group and Function
  Time% |      Time |     Imb. |  Imb. |    Calls | Group
        |           |     Time | Time% |          |  Function
        |           |          |       |          |   PE=HIDE
        |           |          |       |          |    Thread=HIDE
 100.0% | 25.786538 |       -- |    -- | 35,083.0 | Total
|-------------------------------------------------------------------------
|  73.3% | 18.898477 |       -- |    -- | 21,113.0 | OACC
||------------------------------------------------------------------------
||  13.5% |  3.491808 | 0.000623 |  0.0% |    200.0 | fluxi_.ACC_SYNC_WAIT@li.92
||  13.1% |  3.378351 | 0.003587 |  0.2% |    200.0 | fluxj_.ACC_SYNC_WAIT@li.108
||  12.9% |  3.338869 | 0.016283 |  1.0% |    200.0 | fluxk_.ACC_SYNC_WAIT@li.105
||   8.2% |  2.124079 | 0.004317 |  0.4% |    200.0 | fluxj_.ACC_COPY@li.32
||   1.4% |  0.360217 | 0.000020 |  0.0% |  1,010.0 | mpicx_.ACC_COPY@li.322
||   8.2% |  2.124079 | 0.004317 |  0.4% |    200.0 | fluxj_.ACC_COPY@li.32
||   8.2% |  2.104135 | 0.005343 |  0.5% |    200.0 | fluxk_.ACC_COPY@li.31
||   4.2% |  1.081927 | 0.000590 |  0.1% |     21.0 | tmstep_
||   3.0% |  0.785531 | 0.001003 |  0.3% |      1.0 | setiv_
||   2.7% |  0.703152 | 0.067870 | 17.6% |    202.0 | parallel_
||   1.9% |  0.482106 | 0.297350 | 76.3% |      1.0 | flowio_
||   1.8% |  0.460976 | 0.066984 | 25.4% |    303.0 | ghost_
||   1.6% |  0.415937 | 0.000363 |  0.2% |    100.0 | analysis_
||========================================================================
|   3.3% |  0.838605 |       -- |    -- |  3,261.0 | MPI
||------------------------------------------------------------------------
||   2.2% |  0.559752 | 0.178772 | 48.4% |      2.0 | MPI_REDUCE
||========================================================================
|   1.0% |  0.263651 | 0.000053 |  0.0% |     13.0 | ETC
||------------------------------------------------------------------------
||   1.0% |  0.263651 | 0.000053 |  0.0% |     13.0 | _END
|========================================================================
```

Notice that the data transfer for the halo exchange now uses very little time

But wait what is this??? We should not have to transfer data inside fluxj and fluxk

So we use CRAY_ACC_DEBUG=2 and rerun

```
ACC: Start transfer 5 items from src/fluxj.f:32
ACC:       allocate, copy to acc 'sjx' (31990464 bytes)
ACC:       allocate, copy to acc 'sjx' (31990464 bytes)
ACC:       allocate, copy to acc 'sjy' (31990464 bytes)
ACC:       allocate, copy to acc 'sjy' (31990464 bytes)
ACC:       allocate, copy to acc 'sjz' (31990464 bytes)
ACC:       allocate, copy to acc 'sjz' (31990464 bytes)
ACC:       allocate <internal> (227672064 bytes)
ACC:       allocate <internal> (147456 bytes)
ACC: End transfer (to acc 95971392 bytes, to host 0 bytes)
```

Didn’t add those arrays into the data map

```
126.                        #ifdef OMP_TARGET
127.                        !$omp declare target (exj2,exj4)
128.  +                     !$omp target data map(tofrom:SIY,VAV,SIX,UAV,SIZ,WAV,QAV,PAV,U,V,W,T,
129.                        !$omp&         Y,W,T11,T21,Q,HF,DS,DS1,T31,TAV,T12,T22,T32,T13,T23,
130.                        !$omp&         T33,HF,DTV,DQ)
131.                        #endif
```

Because they are used down the call chain in VICJ

```
511.    V
512.    V                        SX = SJX(I,J,K)
513.    V                        SY = SJY(I,J,K)
514.    V                        SZ = SJZ(I,J,K)
515.    V
516.    V                        FSJ(I,J,2) = FSJ(I,J,2) + TXX * SX + TXY * SY + TXZ * SZ
517.    V                        FSJ(I,J,3) = FSJ(I,J,3) + TYX * SX + TYY * SY + TYZ * SZ
518.    V                        FSJ(I,J,4) = FSJ(I,J,4) + TZX * SX + TZY * SY + TZZ * SZ
519.    V                        FSJ(I,J,5) = FSJ(I,J,5) +
520.    V                     >                (TXX*UAVE + TXY*VAVE + TXZ*WAVE + QX) * SX +
521.    V                     >                (TYX*UAVE + TYY*VAVE + TYZ*WAVE + QY) * SY +
522.    V                     >                (TZX*UAVE + TZY*VAVE + TZZ*WAVE + QZ) * SZ
523.    V---------------->       ENDDO
```

There - those went away

```
Table 1:  Profile by Function Group and Function
  Time% |      Time |     Imb. |  Imb. |    Calls | Group
        |           |     Time | Time% |          |  Function
        |           |          |       |          |   PE=HIDE
        |           |          |       |          |    Thread=HIDE
 100.0% | 21.612385 |       -- |    -- | 35,083.0 | Total
|-----------------------------------------------------------------------
|  68.0% | 14.693815 |       -- |    -- | 21,113.0 | OACC
||----------------------------------------------------------------------
||  16.2% |  3.494655 | 0.000677 |  0.0% |    200.0 | fluxi_.ACC_SYNC_WAIT@li.92
||  15.6% |  3.380081 | 0.001161 |  0.1% |    200.0 | fluxi_.ACC_SYNC_WAIT@li.108
||   2.7% |  0.580301 | 0.006628 |  2.3% |      1.0 | les3d_.ACC_COPY@li.409
||   2.0% |  0.438281 | 0.008003 |  3.6% |      1.0 | les3d_.ACC_COPY@li.216
||======================================================================
|  26.7% |  5.778250 |       -- |    -- | 10,687.0 | USER
||----------------------------------------------------------------------
||   5.8% |  1.253559 | 0.018548 |  2.9% |      1.0 | grid_
||   5.0% |  1.085428 | 0.001729 |  0.3% |     21.0 | tmstep_
||   3.7% |  0.804346 | 0.024287 |  5.9% |      1.0 | setiv_
||   3.0% |  0.640157 | 0.070052 | 19.7% |    202.0 | parallel_
||   2.3% |  0.506806 | 0.070618 | 24.5% |    303.0 | ghost_
||   2.2% |  0.475394 | 0.290094 | 75.8% |      1.0 | flowio_
||   1.9% |  0.416498 | 0.001701 |  0.8% |    100.0 | analysis_
||======================================================================
|   4.1% |  0.876445 |       -- |    -- |  3,261.0 | MPI
||----------------------------------------------------------------------
||   2.6% |  0.556783 | 0.176866 | 48.2% |      2.0 | MPI_REDUCE
||======================================================================
|   1.2% |  0.263798 | 0.000062 |  0.0% |     13.0 | ETC
||----------------------------------------------------------------------
||  1.2% |  0.263798 | 0.000062 |  0.0% |     13.0 | _END
|======================================================================
```

These copies in les3d do the initialization of the GPU and bring the results back at the end

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
```

Much easier to code

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

Timings of various version of Leslie3D on four nodes

	original 64 MPI Tasks	Initial Port 4 MPI Tasks>	Raising Data Region x 4	Halo Packing on GPU x 4
fluxi	2.7	63.1	2.05	2.05
fluxj	2.4	57.3	2.12	2.12
fluxk	2.6	57.3	2.76	2.07
update	0.72	9.4	0.24	0.24
leslie3d	2.52	2.6	14.81	3.49
parallel	0.94	1.2	1.04	1.04
tmstep	0.62	1.1	0.78	1
Total	12.5	192	23.8	12.01

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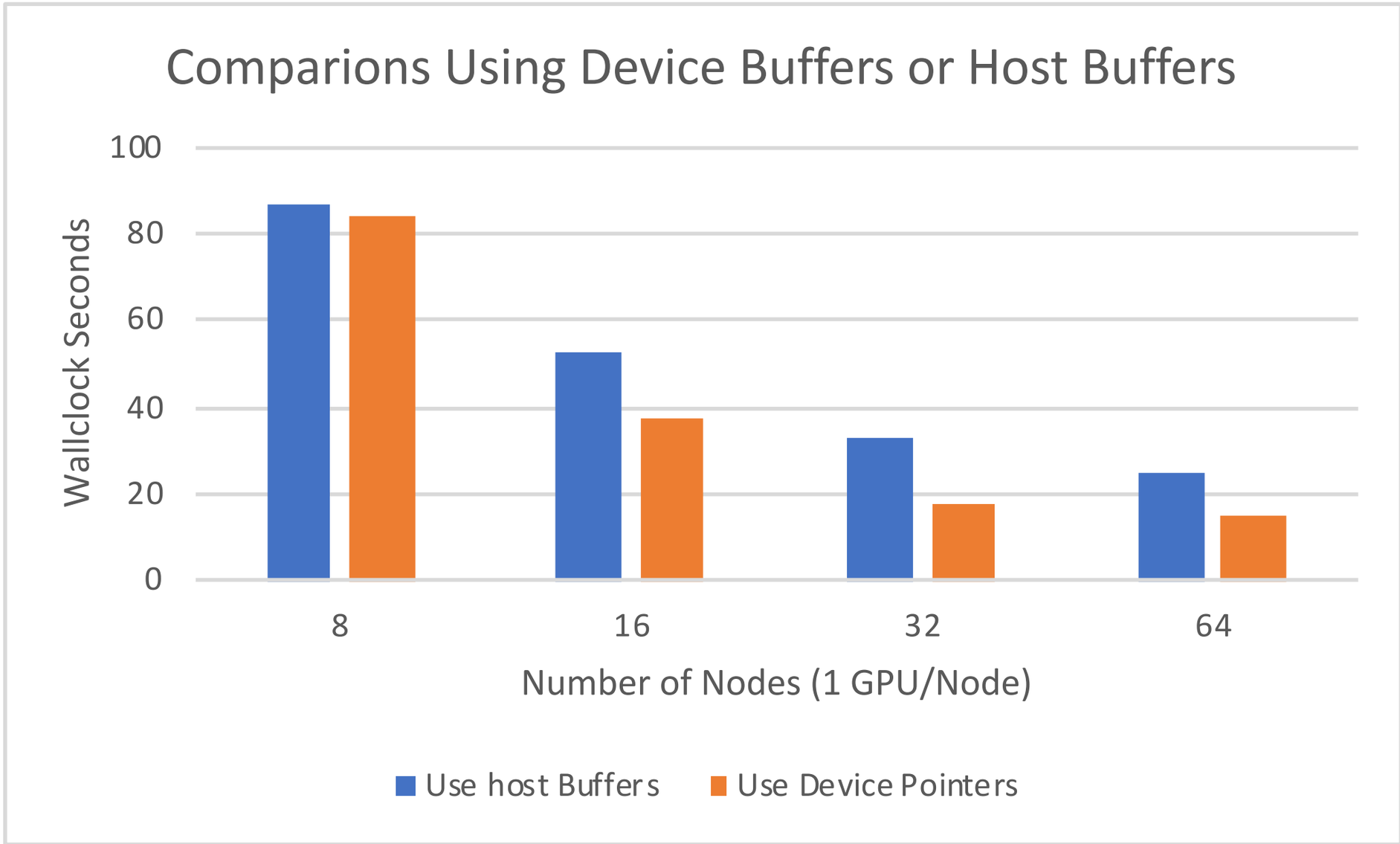
leslie3d	2.52	2.6	14.81	3.49
parallel	0.94	1.2	1.04	1.04
tmstep	0.62	1.1	0.78	1
Total	12.5	192	23.8	12.01

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
```

Now we need to work on the kernels

- We are barely beating the two socket node even with all the work we did.
- The kernels are not optimal, they need some work
- This is left as an exercise for the student

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


Questions?
CRAY