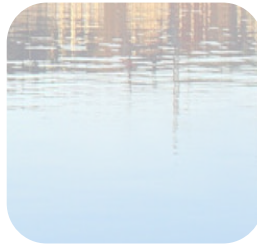


CRAY



## Applying the “Whack-a-Mole” Method Using Cray’s Perftools for Identifying the Moles

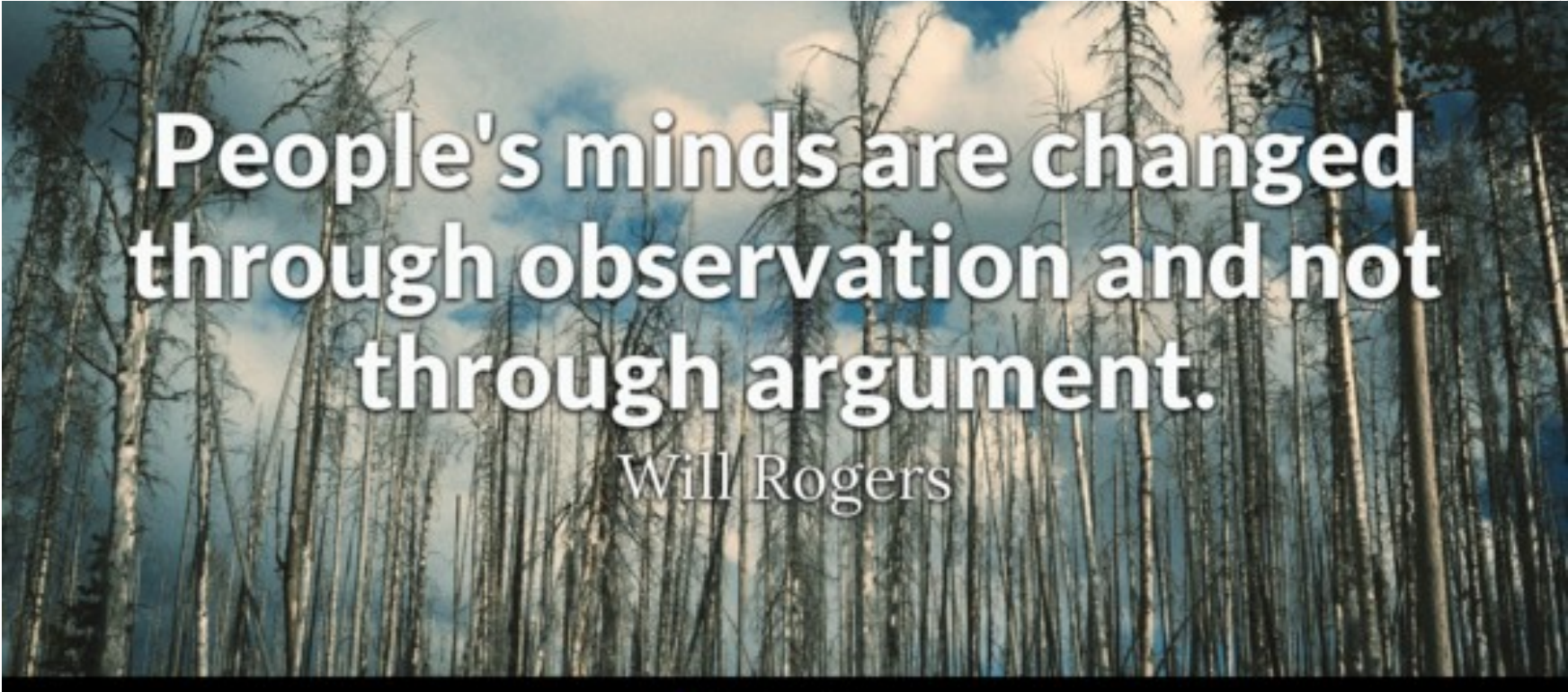
John Levesque, Cray Inc.  
Heidi Poxon, Cray Inc.



# Outline



- **What is the “Whack-a-mole” process?**
- **Short introduction to perftools-lite**
- **Applications to be examined**
  - UMT
  - Leslie3d
  - VH1

The background of the slide is a photograph of a forest with tall, thin trees and a blue sky with clouds. Overlaid on this image is a large, white, bold quote.

**People's minds are changed  
through observation and not  
through argument.**

Will Rogers

# Cray Performance Tools

- **Reduce the time investment associated with porting and tuning applications on Cray systems**
- **Analyze whole-program behavior across many nodes to identify critical performance bottlenecks within a program**
- **Improve your profiling experience by using simple (lite mode) and/or advanced interfaces for a wealth of capability that targets analyzing large HPC jobs**





# Interfaces Available

- **Simple interface (perftools-lite modes) for convenience**
- **Advanced interface (perftools) for in-depth performance investigation and tuning assistance as well as data collection control**
- **Both offer:**
  - Whole program analysis across many nodes
  - Indication of causes of problems
  - Ability to easily switch between the two interfaces



# Used in this Tutorial

- **Several simple modes: `perftools-lite`, `perftools-lite-loops`, `perftools-lite-hbm`**
  - Simply load the desired module, compile, and execute program
- **Additional reports (`pat_report -O calltree`, etc.)**
- **`perftools` advanced interface**
  - Load `perftools` module and build program
  - Instrument program with `pat_build -u -g mpi`
  - Execute instrumented program
  - Create performance reports with `pat_report`
- **Cray compiler (CCE) listing generated by `-hlist=a`**
- **Reveal**
- **Levesque's and Heidi's bag of tricks**

# Applying a “Whack-a-mole” Method Using Cray’s perftools to Identify the Moles



- Ricky Kendal used the phase extensively
- The *Mole* is the most time consuming process in the application
- *Whacking* it means you optimize the process so it no longer takes the most time

# Ricky Kendall 1961 - 2014



- John met Ricky in 1993 when he visited APR to evaluate **FORGE**
  - Taught him to use “.” in vi
- Worked extensively with Ricky for many years at ORNL (AUG 2005 – 2014)



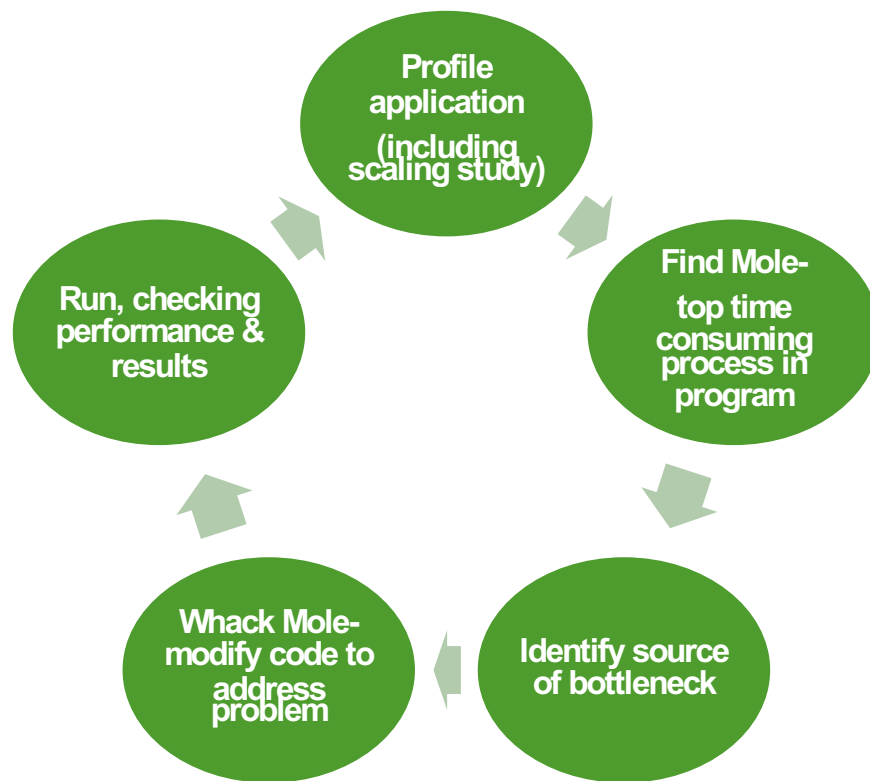
# Whack-a-mole Process



- **Profile your *working* application**
  - On the problem of interest at the scale of interest
  - Don't think you know where the mole is and more importantly why it's the most important bottleneck in the program
  - Performance on a single node is *not* necessarily representative of performance on 1000 nodes

Unless everything scales,  
routines that scale will not be  
important at 1000 nodes

# Whack-a-mole Process (continued)



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# Using the Process on Real Applications

**UMT**

**Leslie3d**

**VH1**



# UMT

The UMT benchmark is a 3D, deterministic,  
multi-group, photon transport code for  
unstructured meshes



Table 1: Tree View

Nesting Level

Head=H

Table 1: Tree View

Nesting Level

Head=H

```
head=HIDE
```

0.0% | 3,971.6 | Total

99.8% | 3,961.9 | main

Inclusive

Inclusive  
Percent of  
Time

Time

```
6| | | | | 66.5% | 2,655.4 | rswpmd_
```

```
7||||| 66.90 | 2,654.7 | snflwxyz_
```

```
8| | | | | | | 22.0% | 872.3 | exchange_
```

```

9||||||| 13.5% | 535.7 | MPI WAIT
0||| 0.5% | 226.5 | MPI_F

```

|   |  |      |       |                     |
|---|--|------|-------|---------------------|
| 9 |  | 8.5% | 336.5 | exchange_exclusive, |
|---|--|------|-------|---------------------|

```
8||||||| 15.6% | 617.7 | snswp3d_
```

```
8||||||| 9.7% | 383.4 | initexchange_
```

```
9| | | | | | | |      |      |      MPI_BARRIER
```

Called From  
snflwxyz\_

```
8 | | | | | | | 6.5% | 260.0 | snmoments_
```

|   | Count | Percentage | Avg Depth | Max Depth | Min Depth | Mean Depth | Stdev Depth | Depth Range | Category       |
|---|-------|------------|-----------|-----------|-----------|------------|-------------|-------------|----------------|
| 8 | 5.8%  | 230.6      | 279.5     | 300.0     | 200.0     | 230.6      | 40.0        | 79.5        | Grav deepy_HSW |

```
8| | | | | | | 4.0% | 160.7 | testfluxconv_
```

```
9| | | | | | | |      |      |      mpi_mpiallreduces_r_$mpif90_m  
10| | | | | | | |     |      |      MPI_ALLREDUCE
```

|    |  |  |  |  |  |  |  |  |   |    |  |  |     |   |  |  |                 |
|----|--|--|--|--|--|--|--|--|---|----|--|--|-----|---|--|--|-----------------|
| 10 |  |  |  |  |  |  |  |  |   |    |  |  |     |   |  |  | MPI_ALLREDUCE   |
| 8  |  |  |  |  |  |  |  |  | 3 | 2% |  |  | 128 | 7 |  |  | setincidentflux |

```
8| | | | | | | | | 3.2% | 128.7 | setincidentflux_
| | | | | | | | |-----
```

```

| | | | | | | | =====
6 | | | | | 21 6% | 859 3 | exchange

```

|   |  |  |  |  |  |       |  |       |  |           |
|---|--|--|--|--|--|-------|--|-------|--|-----------|
| 6 |  |  |  |  |  | 21.6% |  | 859.3 |  | exchange_ |
|   |  |  |  |  |  |       |  |       |  |           |

```

|||||||-----
7||||||| 15.6% | 620.0 | MPI WAIT

```

```
7||||| 15.6% | 620.0 | MPI_WAIT
7||||| 6.0% | 239.3 | exchange (exclusive)
```

|||||| =====

5.0% | 198.1 | rtstrtsn\_

routine-

106.9 | rtstrtsn\_(exclusive)

|      |  |                  |
|------|--|------------------|
| 90.1 |  | __cray_dcopy_HSW |
|------|--|------------------|

=====

of Time 115.2 | advancert\_

\_\_\_\_\_

```
6||||| 1.5% | 60.0 | advancert_(exclusive)
```

```
6||||| 1.4% | 55.2 | snmoments
```

```
|||||=====
||      1.0% |      40.9 | initialize
```

```
||      1.0% |      40.9 | initialize
|
```

---

Leaf child routine-  
Exclusive  
Percent of Time

(exclusive)

MPI\_BARRIER

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# Obtaining a Calltree

- Run `pat_report` with different options after collecting data with `perftools-lite` to get different views of the performance data
- For a calltree:

```
$ pat_report -O calltree exp_dir > rpt.calltree
```



# Plan of Attack – Run Weak/Strong Scaling Study



Problem size: X

Run 8 MPI tasks on 8 nodes,  
vary OpenMP threads from 1 to 32

Problem size: 2X

Run 16 MPI tasks on 16 nodes,  
vary OpenMP threads from 1 to 32

Problem size: 4X

Run 32 MPI tasks on 32 nodes,  
vary OpenMP threads from 1 to 32

Problem size: 4X

64 MPI tasks (1-32 OpenMP threads),  
128 MPI tasks (1-16 OpenMP threads),  
256 MPI tasks (1-8 OpenMP threads),  
512 MPI tasks (1-4 OpenMP threads)

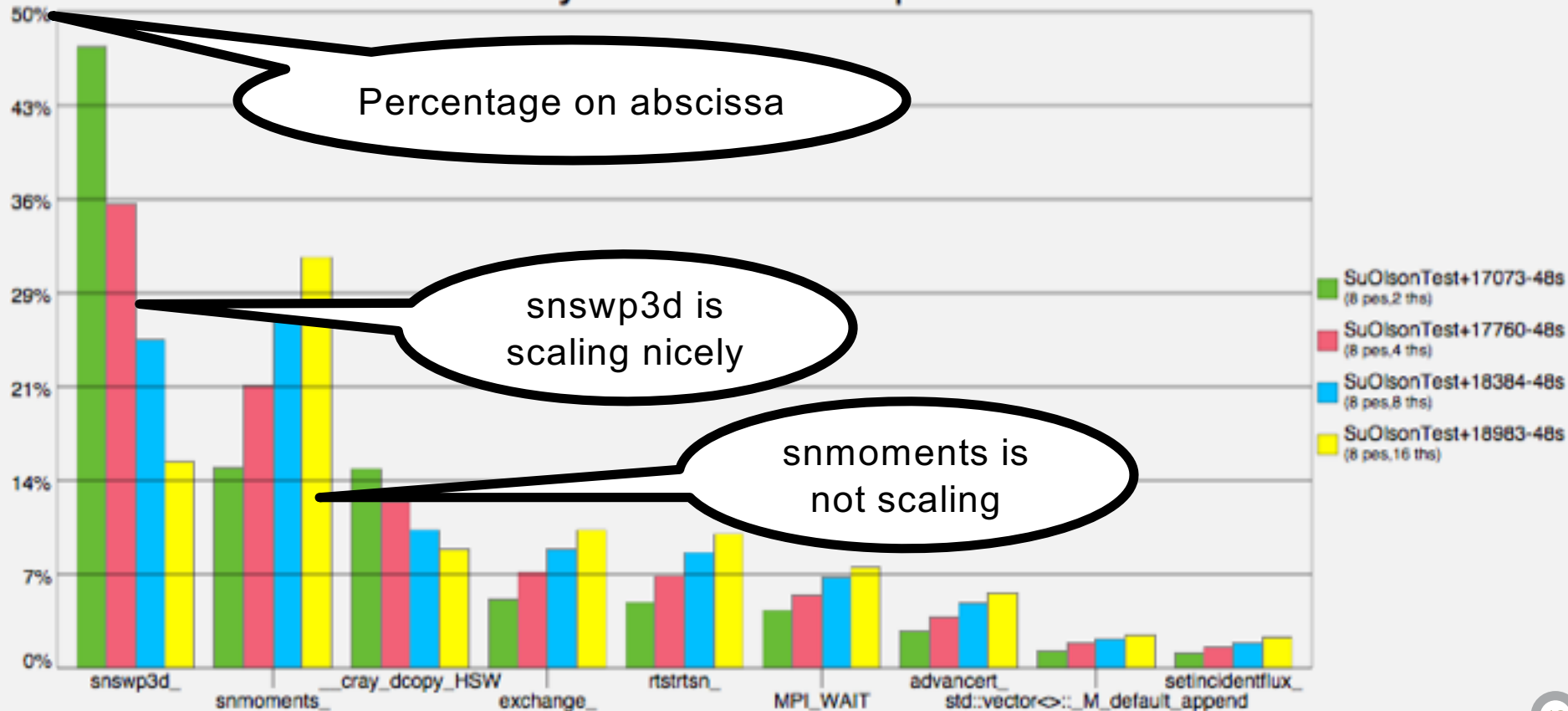
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# UMT Scaling with MPI Tasks and OpenMP Threads

Routines by Percent of Samples



# Observations



- **OpenMP on the node is not doing well above 4 threads**
  - Need to find out why
- **MPI scaling is good, however**
  - At higher MPI counts threading slows down the application

# Using Listing: Existing OpenMP in SNSWP3D

```
105. 1 2 M-----< !$OMP PARALLEL DO PRIVATE(Angle,mm,thnum)
106. + 1 2 M m---<      AngleLoop: do mm=1,NangBin
107. 1 2 M m
108.      Angle = QuadSet% AngleOrder(mm,binSend)
109.      thnum = 1
110.      thnum = OMP_GET_THREAD_NUM() + 1
111. 1 2 M m
112. 1 2 M m      !      Set angular fluxes for reflected angles
113. 1 2
114. + 1 2      Threaded loop      call snreflect(Angle, PSIB)
115. 1 2 M m
116. 1 2 M m      !      Sweep the mesh, calculating PSI for each corner; the
117. 1 2 M m      !      boundary flux array PSIB is also updated here.
118. 1 2 M m      !      Mesh cycles are fixed automatically.
119. 1 2 M m
120. + 1 2 M m      call snswp3d(Groups, Angle,                                &
121. 1 2 M m      QuadSet%next(1,Angle),QuadSet%nextZ(1,Angle),                &
122. 1 2 M m      PSI(1,1,Angle),PSIB(1,1,Angle))
123. 1 2 M m
124. 1 2 M m-->>      enddo AngleLoop
```

Threaded Region

Threaded loop

Outer Loop of Nest

# SNMOMENTS is Not Threaded



```
55.
56.  AC-----<>    Phi(:, :) = zero
57.
58.  + 1-----<    AngleLoop, Angle=1, QuadSet%NumAngles
59.    1
60.    1              quadwt = QuadSet% Weight(Angle)
61.    1
62.    1              if (quadwt /= zero) then
63.    1
64.  + 1 2-----<    do ic=1,ncornr
65.    1 2 Vr2--<    do ig=1,Groups
66.    1 2 Vr2        Phi(ig,ic) = Phi(ig,ic) + quadwt*psic(ig,ic,Angle)
67.    1 2 Vr2-->    enddo
68.    1 2----->    enddo
69.    1
70.    1              endif
71.
72.  ----->    enddo AngleLoop
73.
    return
  end subroutine snmoments
```

When nesting level contains number – no parallelism or vectorization

+ indicates a comment

V – Vectorized  
r2 – unrolled by 2

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# Obtaining a Listing

- CCE provides loopmark, cross-references, compile options, and optimization messages in easy-to-read text files
- Just add the following CCE flag to Makefile:

```
-h list=a ...
```

- Tip: For additional information on restructuring and optimization changes made by CCE, try `-h list=d` for decompiled code

# Before Adding Loop-level Parallelism



- **Determine loop lengths by using perftools-lite-loops**
  - **Can only use when existing OpenMP in program is disabled**
    - perftools-lite disables OpenMP in CCE for the experiment
  - Remember that loops can change with job size (as MPI ranks increase)

Load perftools-lite-loops module

Build and run

View batch job output file or lite report in expdir/rpt-files/RUNTIME.rpt

# UMT Loop Profile (perftools-lite-loops)

Remember there is no  
threading in these  
samples

CRAY

Table 1: Inclusive and Exclusive Time in Loops (from -hprofile\_generate)

|       |       |  | Loop Hit  | Loop  | Loop  | Loop      | Function=/.LOOP[.]       |
|-------|-------|--|-----------|-------|-------|-----------|--------------------------|
|       |       |  |           | Trips | Trips | Trips     | PE=HIDE                  |
|       |       |  |           | Avg   | Min   | Max       |                          |
| ----- |       |  |           |       |       |           |                          |
|       | 98.9% |  | 1         | 7.0   | 7     | 7         | main.LOOP.1.1i.11        |
|       | 92.4% |  | 7         | 4.7   | 3     | 5         | rtmainsn_.LOOP.1.1i.9    |
|       | 92.2% |  | 33        | 1.0   | 1     | 1         | rtmainsn_.LOOP.2.1i.159  |
|       | 92.1% |  | 33        | 1.0   | 1     | 1         | rtmainsn_.LOOP.3.1i.167  |
|       | 71.6% |  | 33        | 1.6   | 1     | 3         | snflwxyz_.LOOP.1.1i.87   |
|       | 59.3% |  | 54        | 6.9   | 4     | 8         | snflwxyz_.LOOP.2.1i.95   |
|       | 44.0% |  | 90        | 10.0  | 10    | 90        | snflwxyz_.LOOP.3.1i.106  |
|       | 41.2% |  | 28        | 10.0  | 10    | 28        | snswp3d_.LOOP.01.1i.78   |
|       | 28.2% |  | 8         | 10.0  | 10    | 8         | snswp3d_.LOOP.04.1i.99   |
|       | 19.1% |  | 8         | 10.0  | 10    | 8         | exchange_.LOOP.06.1i.120 |
|       | 19.1% |  | 6         | 10.0  | 10    | 6         | exchange_.LOOP.07.1i.121 |
|       | 14.0% |  | 3         | 10.0  | 10    | 3         | snswp3d_.LOOP.06.1i.136  |
|       | 11.9% |  | 400       | 10.0  | 10    | 400       | snswp3d_.LOOP.05.1i.110  |
|       | 8.2%  |  | 8         | 10.0  | 10    | 8         | exchange_.LOOP.08.1i.132 |
|       | 8.0%  |  | 8         | 10.0  | 10    | 8         | exchange_.LOOP.09.1i.134 |
|       | 6.9%  |  | 405       | 10.0  | 10    | 405       | snswp3d_.LOOP.05.1i.110  |
|       | 6.9%  |  | 2,025     | 1.6   | 1     | 8         | exchange_.LOOP.01.1i.71  |
|       | 5.8%  |  | 7,499,520 | 3.0   | 3     | 7,499,520 | snmoments_.LOOP.1.1i.58  |
|       | 5.0%  |  | 40        | 720.0 | 720   | 40        | snmoments_.LOOP.2.1i.64  |
|       | 5.0%  |  | 28,800    | 224.0 | 224   | 28,800    | snmoments_.LOOP.3.1i.65  |
|       | 4.9%  |  | 6,451,200 | 400.0 | 400   | 6,451,200 | snmoments_.LOOP.3.1i.65  |
|       | 4.7%  |  | 405       | 1.6   | 1     | 8         | exchange_.LOOP.01.1i.71  |

Ordered by loops that  
take most of the time

This is the loop  
with OpenMP

snmoments has nice  
loops lengths



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# Profile Loops with Call Tree (1 of 2)

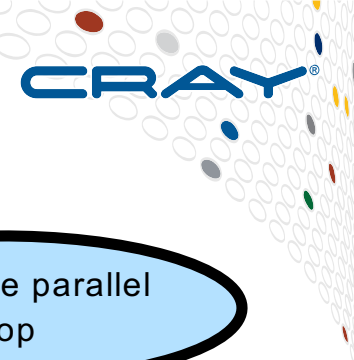
Table 1: Function Calltree View

| Time%   | Time      | Calls     | Calltree                      |
|---------|-----------|-----------|-------------------------------|
|         |           |           | PE=HIDE                       |
| 100.0%  | 57.147586 | --        | Total                         |
| -----   |           |           |                               |
| 100.0%  | 57.147550 | 2.0       | main                          |
| 98.9%   | 56.543299 | --        | main.LOOP.1.li.189            |
| 3       |           |           | advance                       |
| 4 98.9% | 56.538457 | --        | Teton<>::cxxRadtr             |
| 5 98.9% | 56.538442 | 7.0       | radtr_                        |
| -----   |           |           |                               |
| 6       | 97.0%     | 55.459264 | 7.0   rtmainasn_              |
| -----   |           |           |                               |
| 7       | 92.5%     | 52.838008 | --   rtmainasn_.LOOP.1.li.149 |
| 8       | 92.3%     | 52.719389 | --   rtmainasn_.LOOP.2.li.159 |
| 9       | 92.1%     | 52.638677 | --   rtmainasn_.LOOP.3.li.167 |
| -----   |           |           |                               |
| 10      | 76.7%     | 43.811029 | 33.0   rswpmd_                |
| 11      | 76.6%     | 43.802991 | 33.0   snflwxyz_              |
| -----   |           |           |                               |
| 12      | 71.6%     | 40.911652 | --   snflwxyz_.LOOP.1.li.87   |
| -----   |           |           |                               |
| 13      | 59.3%     | 33.883425 | --   snflwxyz_.LOOP.2.li.95   |
| -----   |           |           |                               |
| 14      | 44.0%     | 25.123658 | --   snflwxyz_.LOOP.3.li.106  |

Remember there is no threading  
in these samples

This is the  
parallel loop

# Profile Loops with Call Tree (2 of 2)



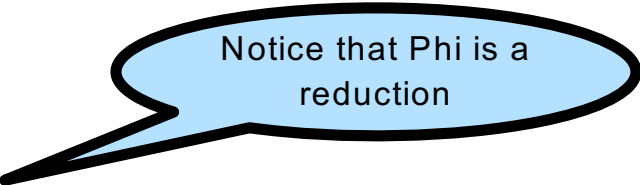
```
14||||| 44.0% | 25.123658 | -- | snflwxyz_.LOOP.3.li.106
15||||| 43.4% | 24.805902 | 33,480.0 | snswp3d_
14||||| 15.3% | 8.759766 | 372.0 | exchange_
|||||=====
13||||| 8.0% | 4.592279 | 54.0 | initexchange_
13||||| 2.9% | 1.654016 | 54.0 | testfluxconv_
13||||| 1.4% | 0.781868 | 54.0 | setincidentflux_
|||||=====
12||||| 4.1% | 2.363264 | 33.0 | snmoments_
|||||=====
10||||| 15.4% | 8.819869 | 33.0 | exchange_
|||||=====
7||||| 3.2% | 1.814788 | 7.0 | rtstrtsn_
|||||-----
8||||| 1.8% | 1.002470 | 7.0 | rtstrtsn_(exclusive)
8||||| 1.4% | 0.812278 | 7.0 | setbdy_
|||||=====
6||||| 1.9% | 1.069855 | 7.0 | advancert_
|=====
```

This is the parallel loop

This is the mole when snflxyz.106 is threaded

# Major Loop in SNMOMENTS (From Listing)

```
56.      AC-----<>      Phi(:, :) = zero
57.
58.  + 1-----<      AngleLoop: do Angle=1, QuadSet%NumAngles
59.      1
60.      1      quadwt = QuadSet% Weight(Angle)
61.      1
62.      1      if (quadwt /= zero) then
63.      1
64.  + 1 2-----<      do ic=1, ncornr
65.      1 2 Vr2--<      do ig=1, Groups
66.      1 2 Vr2      Phi(ig, ic) = Phi(ig, ic) + quadwt*psic(ig, ic, Angle)
67.      1 2 Vr2-->      enddo
68.      1 2----->      enddo
69.      1
70.      1      endif
71.      1
72.      1----->      enddo AngleLoop
```

A blue speech bubble with a black outline, pointing towards the line of code where Phi is updated. It contains the text "Notice that Phi is a reduction".

Notice that Phi is a reduction



# Questions About This Loop Nest

- Do we want to parallelize on ANGLE?
- How do we handle a reduction operation on an array?
  - This could be inefficient, or at least less efficient than parallelizing on a different loop

# Reductions On An Array Are An Issue

This information is obtained from a perftools-lite-loops run:

|      |          |          |           |       |     |     |                         |
|------|----------|----------|-----------|-------|-----|-----|-------------------------|
| 5.0% | 2.864861 | 0.003020 | 40        | 720.0 | 720 | 720 | snmoments_.LOOP.1.li.58 |
| 5.0% | 2.861841 | 0.051047 | 28,800    | 224.0 | 224 | 224 | snmoments_.LOOP.2.li.64 |
| 4.9% | 2.810795 | 2.810795 | 6,451,200 | 400.0 | 400 | 400 | snmoments_.LOOP.3.li.65 |

```
56.    AC-----<>      Phi(:, :) = zero
57.    MV-----< !OMP PARALLEL DO PRIVATE(angle,quadwt,ic,ig) reduction(+:PHI(:400,:224))
58. + MV m-----<      AngleLoop: do Angle=1,QuadSet%NumAngles
59.    MV m
60.    MV m              quadwt = QuadSet% Weight(Angle)
61.    MV m
62.    MV m              if (quadwt /= zero) then
63.    MV m
64. + MV m 3-----<          do ic=1,ncornr
65.    MV m 3 Vr2--<          do ig=1,Groups
66.    MV m 3 Vr2          Phi(ig,ic) = Phi(ig,ic) + quadwt*psic(ig,ic,Angle)
67.    MV m 3 Vr2-->          enddo
68.    MV m 3----->          enddo
69.    MV m
70.    MV m              endif
71.    MV m
72.    MV m----->>      enddo AngleLoop
```



These do not need to  
be constant in new  
OpenMP standard



# Parallelizing a Different Loop

```
56.      AC-----<>      Phi(:, :) = zero
57.      M-----<  !$OMP PARALLEL DO PRIVATE(ic,angle,quadwt,ig)
58.  + M m-----<      CornerLoop: do ic=1,ncornr
59.  + M m 3-----<      AngleLoop: do Angle=1,QuadSet%NumAngles
60.      M m 3
61.      M m 3      quadwt = QuadSet% Weight(Angle)
62.      M m 3
63.      M m 3      if (quadwt /= zero) then
64.      M m 3
65.      M m 3 Vr2--<      do ig=1,Groups
66.      M m 3 Vr2      Phi(ig,ic) = Phi(ig,ic) + quadwt*psic(ig,ic,Angle)
67.      M m 3 Vr2-->      enddo
68.      M m 3
69.      M m 3      endif
70.      M m 3
71.      M m 3----->      enddo AngleLoop
72.      M m----->>      enddo CornerLoop
```

Pull the ic loop outside  
the angle loop...

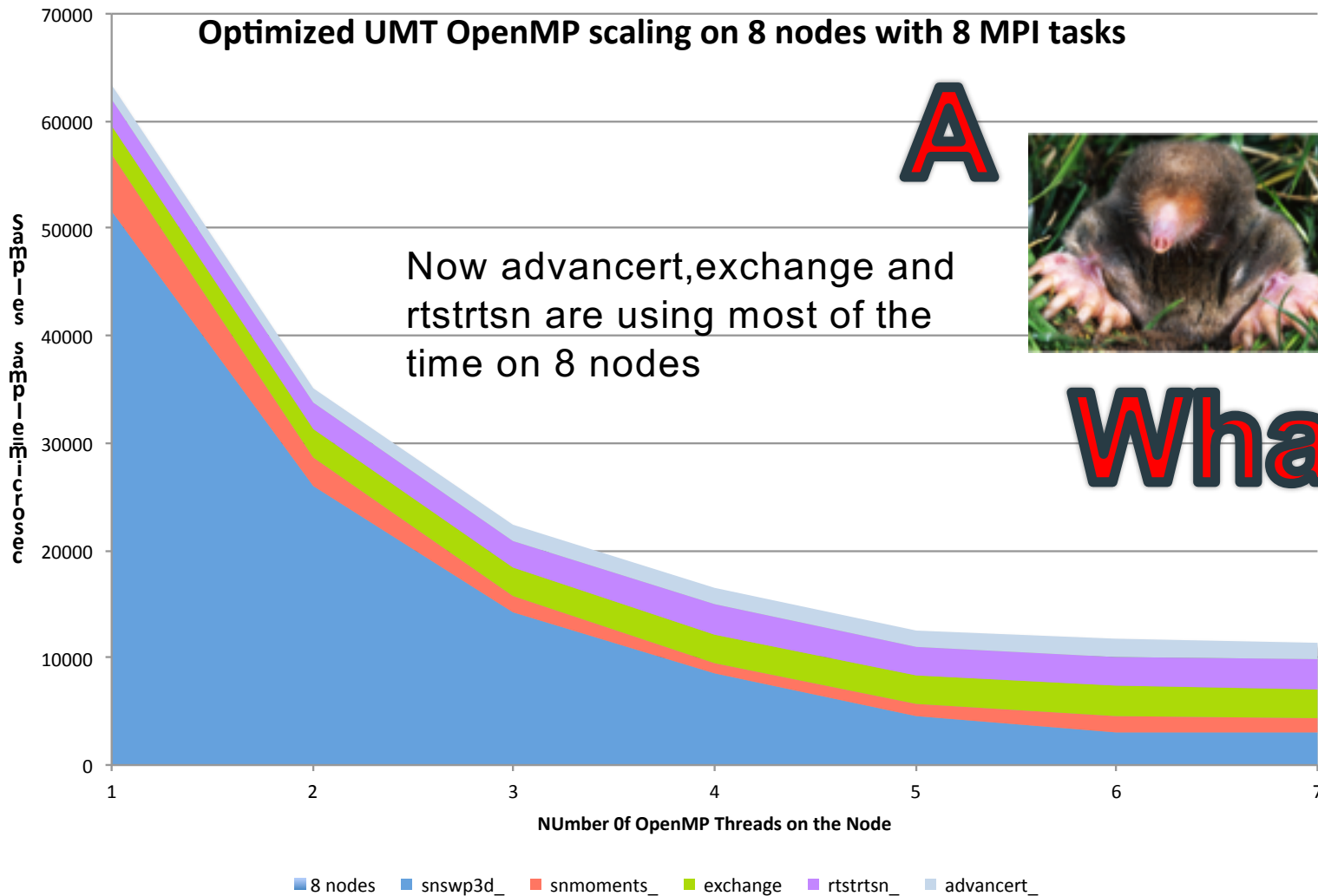
# Optimized UMT OpenMP scaling on 8 nodes with 8 MPI tasks

**A**



Now advancert,exchange and  
rtstrtsn are using most of the  
time on 8 nodes

**Whacked**





# Major Loop in RTSTRTSN

```
51.  + F-----<
52.    F I
53.    F
54.    F
55.  + F 2-----<
56.    F 2 C-----<
57.    F 2 C VCr2----<>
58.    F 2 C----->
59.    F 2----->
60.    F----->
```

```
ZoneLoop: do zone=1,nzones
  Z => getZoneData(Geom, zone)
  nCorner = Z% nCorner
  c0      = Z% c0
  do ia=1,Size%nangSN
    do c=1,nCorner
      Z% STime(:,c,ia) = tau*psir(:,c0+c,ia)
    enddo
  enddo
enddo ZoneLoop
```



# Parallelized Using OpenMP

```
51.      M-----< !$OMP PARALLEL DO PRIVATE(zone,nCorner,c0,ia,c)
52. + M mF-----<      ZoneLoop: do zone=1,nzones
53.      M mF I          Z => getZoneData(Geom, zone)
54.      M mF          nCorner = Z% nCorner
55.      M mF          c0      = Z% c0
56. + M mF 3-----<      do ia=1,Size%nangSN
57.      M mF 3 C-----<          do c=1,nCorner
58.      M mF 3 C VCr2-----<>          Z% STime(:,c,ia) = tau*psir(:,c0+c,ia)
59.      M mF 3 C----->          enddo
60.      M mF 3----->      enddo
61.      M mF----->>      enddo ZoneLoop
```

For the zone loop, the average length is 824 on 8 MPI Tasks and only 14 when using 512 MPI Tasks

# One of Two Major Loops in Exchange

```
88.      1 2      ! Loop over exiting angle, boundary element pairs for this communicat
89.      1 2
90.  + 1 2 3-----<      do ia=1,NangBin
91.      1 2 3      Angle = QuadSet% AngleOrder(ia,bin)
92.      1 2 3      nsend = Comm% nsend(ia)
93.      1 2 3
94.  + 1 2 3 4-----<      do i=1,nsend
95.      1 2 3 4
96.      1 2 3 4      ib = Comm% ListSend(nsend0+i)
97.      1 2 3 4
98.  + 1 2 3 4 Vpr2-----<      do ig=1,ngroups
99.      1 2 3 4 Vpr2      Comm% psibsend(message+ig) = psib(ig,ib,Angle)
100.     1 2 3 4 Vpr2----->      enddo
101.     1 2 3 4
102.     1 2 3 4      message = message + ngroups
103.     1 2 3 4
104.     1 2 3 4----->      enddo
105.     1 2 3      nsend0 = nsend0 + nsend
106.     1 2 3----->      enddo
```

# Some Major Problems with This Exchange Loop

- **message** and **send0** illustrate loop carried dependencies
- Must restructure to enable parallelization

# Exchange Loop Restructured & Parallelized

```

93.      1 2                ! scalar setup loop
94.  + 1 2 r4-----<      do ia=1,NangBin
95.    1 2 r4                vmmessage(ia) = message
96.    1 2 r4                vnsend0(ia) = nsend0
97.    1 2 r4                nsend = Comm% nsend(ia)
98.    1 2 r4                message = message + nsend * ngroups
99.    1 2 r4                nsend0 = nsend0 + nsend
100.   1 2 r4----->      enddo

101.      1 2
102.    1 2 M-----< !$OMP PARALLEL DO PRIVATE(IA,Angle,nsend,i,ib,ig,message,nsend0)
103.  + 1 2 M m-----<      do ia=1,NangBin
104.    1 2 M m                message = vmmessage(ia)
105.    1 2 M m                nsend0 = vnsend0(ia)
106.    1 2 M m
107.    1 2 M m                Angle = QuadSet% AngleOrder(ia,bin)
108.    1 2 M m                nsend = Comm% nsend(ia)
109.    1 2 M m
110.  + 1 2 M m 5-----<      do i=1,nsend
111.    1 2 M m 5
112.    1 2 M m 5                ib = Comm% ListSend(nsend0+i)
113.    1 2 M m 5
114.  + 1 2 M m 5 Vpr2-----<      do ig=1,ngroups
115.    1 2 M m 5 Vpr2          Comm% psibsend(message+ig) = psib(ig,ib,Angle)
116.    1 2 M m 5 Vpr2----->      enddo
117.    1 2 M m 5
118.    1 2 M m 5                message = message + ngroups
119.    1 2 M m 5
120.    1 2 M m 5----->      enddo
121.    1 2 M m                nsend0 = nsend0 + nsend
122.    1 2 M m----->>      enddo
    
```



# Major Loop in AdvanceRT

```
136.      Fr2 I              Z      => getZoneData(Geom, zone)
137.      Fr2
138.      Fr2              nCorner = Z% nCorner
139.      Fr2              c0      = Z% c0
140.      Fr2              PhiAve  = zero
141.      Fr2
142.  + Fr2 2-----<      do c=1,nCorner
143.      Fr2 2              volumeRatio = Z% VolumeOld(c)/Z% Volume(c)
144.      Fr2 2 Vr2-----<>      Phi(:,c0+c) = Phi(:,c0+c)*volumeRatio
145.      Fr2 2
146.  + Fr2 2 3-----<      do ia=1,numAngles
147.      Fr2 2 3 Vr2-----<>      psir(:,c0+c,ia) = psir(:,c0+c,ia)*volumeRatio
148.      Fr2 2 3----->      enddo
149.      Fr2 2
150.      Fr2 2              sumRad = zero
151.      Fr2 2 Vr4-----<      do ig=1,ngr
152.      Fr2 2 Vr4              sumRad = sumRad + Phi(ig,c0+c)
153.      Fr2 2 Vr4----->      enddo
154.      Fr2 2
155.      Fr2 2              PhiAve = PhiAve + Z% Volume(c)*sumRad
156.      Fr2 2
157.      Fr2 2----->      enddo
```

# AdvanceRT Loop Parallelized with OpenMP



```
134. + F-----<      ZoneLoop2: do zone=1,nzones
135.      F
136.      F M-----< !$OMP PARALLEL PRIVATE(c,volumeRatio,ia,sumRad,ig)
137.      F M I          Z          => getZoneData(Geom, zone)
138.      F M
139.      F M          nCorner = Z% nCorner
140.      F M          c0      = Z% c0
141.      F M          PhiAve = zero
142.      F M          !$OMP DO REDUCTION(+:PhiAve)
143. + F M m-----<      do c=1,nCorner
144.      F M m          volumeRatio = Z% VolumeOld(c)/Z% Volume(c)
145.      F M m Vr2-----<>      Phi(:,c0+c) = Phi(:,c0+c)*volumeRatio
146.      F M m
147. + F M m 4-----<      do ia=1,numAngles
148.      F M m 4 Vr2-----<>          psir(:,c0+c,ia) = psir(:,c0+c,ia)*volumeRatio
149.      F M m 4----->      enddo
150.      F M m
151.      F M m          sumRad = zero
152.      F M m Vr4-----<      do ig=1,ngr
153.      F M m Vr4          sumRad = sumRad + Phi(ig,c0+c)
154.      F M m Vr4----->      enddo
155.      F M m
156.      F M m          PhiAve = PhiAve + Z% Volume(c)*sumRad
157.      F M m
158.      F M m----->      enddo
159.      F M-----> !$OMP END PARALLEL
```

Z is a pointer in a module and it must be made threadprivate and set by all threads



# 8 Node Configuration

Original

Optimized

CRAY

Table 1: Profile by Function

| Samp%  | Samp     | Imb.  | Imb.  | Group             |
|--------|----------|-------|-------|-------------------|
|        |          | Samp  | Samp% | Function=[MAX10]  |
|        |          |       |       | PE=HIDE           |
|        |          |       |       | Thread=HIDE       |
| 100.0% | 27,861.2 | --    | --    | Total             |
| 79.4%  | 22,111.1 | --    | --    | USER              |
| 27.0%  | 7,508.6  | 66.4  | 1.0%  | snmoments_        |
| 23.2%  | 6,453.2  | 73.8  | 1.3%  | snswp3d_          |
| 9.5%   | 2,636.0  | 23.0  | 1.0%  | exchange_         |
| 8.9%   | 2,488.8  | 24.2  | 1.1%  | rtstrtsn_         |
| 4.9%   | 1,378.6  | 6.4   | 0.5%  | advancert_        |
| 2.2%   | 619.4    | 66.6  | 11.1% | double* std::__un |
| 2.0%   | 561.4    | 8.6   | 1.7%  | setincidentflux_  |
| 11.6%  | 3,219.2  | --    | --    | ETC               |
| 10.8%  | 3,011.9  | 107.1 | 3.9%  | __cray_dcopy_HSW  |
| 9.0%   | 2,518.9  | --    | --    | MPI               |
| 7.3%   | 2,033.1  | 184.9 | 9.5%  | MPI_WAIT          |

Table 1: Profile by Function

| Samp%  | Samp     | Imb. | Imb.  | Group                  |
|--------|----------|------|-------|------------------------|
|        |          | Samp | Samp% | Function=[MAX10]       |
|        |          |      |       | PE=HIDE                |
|        |          |      |       | Thread=HIDE            |
| 100.0% | 15,762.0 | --   | --    | Total                  |
| 67.6%  | 10,658.9 | --   | --    | USER                   |
| 41.3%  | 6,509.0  | 37.0 | 0.6%  | snswp3d_               |
| 5.8%   | 917.6    | 10.4 | 1.3%  | snmoments_.LOOP@li.58  |
| 3.9%   | 620.6    | 65.4 | 10.9% | double* std::__uninit  |
| 3.5%   | 557.4    | 8.6  | 1.7%  | setincidentflux_       |
| 3.5%   | 551.4    | 2.6  | 0.5%  | rtstrtsn_.LOOP@li.51   |
| 2.2%   | 350.4    | 5.6  | 1.8%  | advancert_.LOOP@li.142 |
| 2.1%   | 338.5    | 16.5 | 5.3%  | exchange_.LOOP@li.103  |
| 2.1%   | 334.6    | 9.4  | 3.1%  | exchange_.LOOP@li.178  |
| 20.1%  | 3,168.6  | --   | --    | ETC                    |
| 18.7%  | 2,949.2  | 94.8 | 3.6%  | __cray_dcopy_HSW       |
| 12.1%  | 1,904.5  | --   | --    | MPI                    |
| 10.5%  | 1,653.0  | 66.0 | 4.4%  | MPI_WAIT               |

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ANALYZE

# Some Results



- **Fastest 8 node configuration:**
  - 8 MPI ranks and 8 threads
- **Fastest 32 node configuration:**
  - 256 MPI tasks and 4 threads on 32 nodes



# 32 Node Configuration

Original      Optimized

CRAY®

Table 1: Profile by Function

| Samp%  | Samp    | Imb.  | Imb.  | Group                                      |
|--------|---------|-------|-------|--------------------------------------------|
|        |         | Samp  | Samp% | Function=[MAX10]<br>PE=HIDE<br>Thread=HIDE |
| 100.0% | 4,015.1 | --    | --    | Total                                      |
| 47.9%  | 1,924.6 | --    | --    | MPI                                        |
| 29.6%  | 1,190.3 | 452.7 | 27.7% | MPI_WAIT                                   |
| 13.4%  | 537.8   | 616.2 | 53.6% | MPI_BARRIER                                |
| 4.7%   | 188.6   | 239.4 | 56.2% | MPI_ALLREDUCE                              |
| 43.8%  | 1,760.5 | --    | --    | USER                                       |
| 14.1%  | 567.9   | 46.1  | 7.5%  | snswp3d_                                   |
| 13.9%  | 558.1   | 166.9 | 23.1% | exchange_                                  |
| 7.5%   | 300.1   | 11.9  | 3.8%  | snmoments_                                 |
| 3.1%   | 124.6   | 41.4  | 25.1% | setincidentflux_                           |
| 2.6%   | 103.6   | 3.4   | 3.2%  | rtstrtsn_                                  |
| 1.4%   | 58.1    | 2.9   | 4.8%  | advancert_                                 |
| 8.0%   | 320.6   | --    | --    | ETC                                        |
| 7.7%   | 310.6   | 51.4  | 14.2% | __cray_dcopy_HSW                           |

Table 1: Profile by Function

| Samp%  | Samp    | Imb.  | Imb.  | Group                                      |
|--------|---------|-------|-------|--------------------------------------------|
|        |         | Samp  | Samp% | Function=[MAX10]<br>PE=HIDE<br>Thread=HIDE |
| 100.0% | 3,651.9 | --    | --    | Total                                      |
| 54.7%  | 1,998.8 | --    | --    | MPI                                        |
| 37.2%  | 1,360.0 | 444.0 | 24.7% | MPI_WAIT                                   |
| 12.3%  | 447.6   | 668.4 | 60.1% | MPI_BARRIER                                |
| 5.1%   | 184.8   | 269.2 | 59.5% | MPI_ALLREDUCE                              |
| 35.6%  | 1,299.8 | --    | --    | USER                                       |
| 15.9%  | 581.5   | 44.5  | 7.1%  | snswp3d_                                   |
| 4.4%   | 161.0   | 60.0  | 27.3% | exchange_.LOOP@li.103                      |
| 4.2%   | 154.4   | 3.6   | 2.3%  | snmoments_.LOOP@li.58                      |
| 3.5%   | 127.8   | 50.2  | 28.3% | setincidentflux_                           |
| 3.0%   | 110.6   | 86.4  | 44.1% | exchange_.LOOP@li.178                      |
| 1.8%   | 67.0    | 2.0   | 2.9%  | rtstrtsn_.LOOP@li.51                       |
| 9.0%   | 328.6   | --    | --    | ETC                                        |
| 8.6%   | 314.5   | 39.5  | 11.2% | __cray_dcopy_HSW                           |



## Not Real Exciting Speedup at 32 Nodes; However, ??

- **Have we looked at everything?**

- Vectorization



- Parallelization



- Memory Utilization



# Memory Bandwidth Metrics with perftools-lite



```
Avg Process Time:          83.99 secs
High Memory:              15,821.3 MiBytes      659.2 MiBytes per PE
Observed CPU clock boost:  118.1 %
Percent cycles stalled:    76.0 %
Vector intensity (packed instr):  14.7 %
Instr per Cycle:           0.38
I/O Write Rate:           2.407172 MiBytes/sec
```

Table 3: Memory Bandwidth by Numanode

| Memory<br>Traffic<br>GBytes | Local<br>Memory<br>Traffic<br>GBytes | Remote<br>Memory<br>Traffic<br>GBytes | Thread<br>Time         | Memory<br>Traffic<br>GBytes<br>/ Sec | Memory<br>Traffic<br>/ Nominal<br>Peak | Numanode<br>PE=HIDE      |
|-----------------------------|--------------------------------------|---------------------------------------|------------------------|--------------------------------------|----------------------------------------|--------------------------|
| 2,164<br>752.57             | 2,162<br>752.39                      | 2.36<br>0.18                          | 83.914890<br>83.916253 | 25.79<br>8.97                        | 33.6%<br>11.7%                         | numanode.0<br>numanode.1 |

# Using perftools-lite-hbm for Memory Traffic Info



Load perftools-lite-hbm module

Build and run

View batch job output file or lite report in `expdir/rpt-files/RUNTIME.rpt`

# Perftools-lite-hbm Results

Table 5: Profile by Group, Function, and Line

| Samp%  | Samp  | Imb.  | Imb.  | MEM_LOAD_UOPS_RETIRED  | RESOURCE_STALLS        | Group                      |               |
|--------|-------|-------|-------|------------------------|------------------------|----------------------------|---------------|
|        |       | Samp  | Samp% | :HIT_LFB:precise=2     | :ANY                   | Function=[MAX10]<br>Source |               |
|        |       |       |       |                        |                        | Line<br>PE=HIDE            |               |
| 100.0% | 862.5 | --    | --    | 89,509,042,630,218,624 | 1,722,469,802,124      | Total                      |               |
| 62.4%  | 537.9 | --    | --    | 56,224,626,618,220,104 | 991,877,756,035        | USER                       |               |
| 31.2%  | 269.1 | --    | --    | 28,464,157,033,148,192 | 608,254,074,506        | snswp3d_                   |               |
| 3      |       |       |       |                        |                        | snswp3d.F90                |               |
| 4      | 9.1%  | 78.2  | 9.8   | 12.7%                  | 8,549,802,421,201,201  | 176,888,912,461            | line.92       |
| 4      | 1.2%  | 10.0  | 6.0   | 42.9%                  | 879,609,303,122,411    | 22,751,971,753             | line.93       |
| 4      | 1.0%  | 9.0   | 3.0   | 28.6%                  | 879,609,302,723,331    | 20,451,617,059             | line.95       |
| 4      | 1.1%  | 9.9   | 7.1   | 47.9%                  | 879,609,302,703,468    | 22,293,446,105             | line.112      |
| 4      | 7.8%  | 67.6  | 12.4  | 17.7%                  | 7,599,824,374,166,244  | 152,716,084,911            | line.128      |
| 4      | 1.4%  | 12.2  | 2.8   | 21.0%                  | 1,337,006,139,902,300  | 27,724,424,302             | line.138      |
| 4      | 1.6%  | 14.1  | 3.9   | 24.6%                  | 1,266,637,396,229,511  | 32,065,385,985             | line.206      |
| 4      | 4.6%  | 39.2  | 8.8   | 20.8%                  | 4,151,755,908,199,040  | 88,460,785,924             | line.229      |
|        | ===== |       |       |                        |                        |                            |               |
|        | 15.3% | 132.2 | --    | --                     | 14,179,301,951,169,120 | 150,304,652,642            | snmoments_    |
| 3      |       |       |       |                        |                        |                            | snmoments.F90 |
| 4      | 15.3% | 132.1 | 5.9   | 4.9%                   | 14,144,117,579,091,356 | 150,152,590,310            | line.66       |
|        | 7.0%  | 60.0  | --    | --                     | 5,207,287,073,618,042  | 105,802,278,732            | exchange_     |
| 3      |       |       |       |                        |                        |                            | exchange.F90  |
| 4      | 5.2%  | 44.9  | 4.1   | 9.6%                   | 3,588,805,956,844,644  | 77,368,597,030             | line.115      |
| 4      | 1.8%  | 15.1  | 2.9   | 18.3%                  | 1,618,481,116,773,398  | 28,433,681,701             | line.190      |



# OMG – ARRAY SYNTAX

```
110.  + F 2 3-----<          do icface=1,ncfaces
111.    F 2 3
112.    F 2 3          afpm(icface) = omega(1)*Z%A_fp(1,icface,c) + &
113.    F 2 3          omega(2)*Z%A_fp(2,icface,c) + &
114.    F 2 3          omega(3)*Z%A_fp(3,icface,c)
115.    F 2 3
116.    F 2 3          icfp      = Z%Connect(1,icface,c)
117.    F 2 3          ib       = Z%Connect(2,icface,c)
118.    F 2 3
119.    F 2 3          if ( afpm(icface) >= zero ) then
120.    F 2 3            sumArea = sumArea + afpm(icface)
121.    F 2 3          else
122.    F 2 3            if (icfp == 0) then
123.    F 2 3 A-----<>              psifp(:,icface) = psib(:,ib)
124.    F 2 3            else
125.    F 2 3 A-----<>              psifp(:,icface) = psic(:,icfp)
126.    F 2 3            endif
127.    F 2 3
128.    F 2 3 Vr4-----<>          src(:,c)  = src(:,c) - afpm(icface)*psifp(:,icface)
129.    F 2 3            endif
130.    F 2 3----->          enddo
```

# ARRAY SYNTAX: Good for the Cyber 205 and CM5, Not Good for Cache Based Systems



# A



# Whacked

```
109.      F 2
110.      F 2 r6-----<          do icface=1,ncfaces
111.      F 2 r6
112.      F 2 r6                    afpm(icface) = omega(1)*Z%A_fp
113.      F 2 r6                    omega(2)*Z%A_fp
114.      F 2 r6                    omega(3)*Z%A_fp
115.      F 2 r6
116.      F 2 r6                    icfp      = Z%Connect(1,icface,c)
117.      F 2 r6                    ib        = Z%Connect(2,icface,c)
118.      F 2 r6
119.      F 2 r6                    if ( afpm(icface) >= zero ) then
120.      F 2 r6                        sumArea = sumArea + afpm(icface)
121.      F 2 r6                    else
122.      F 2 r6 Vr2-----<          do ig = 1, Groups
123.      F 2 r6 Vr2                    if (icfp == 0) then
124.      F 2 r6 Vr2                        psifp(ig,icface) =
125.      F 2 r6 Vr2                        else
126.      F 2 r6 Vr2                        psifp(ig,icface) =
127.      F 2 r6 Vr2                        endif
128.      F 2 r6 Vr2
129.      F 2 r6 Vr2                        src(ig,c) = src(ig,c)
130.      F 2 r6 Vr2----->                    enddo
131.      F 2 r6                    endif
132.      F 2 r6----->          enddo
```

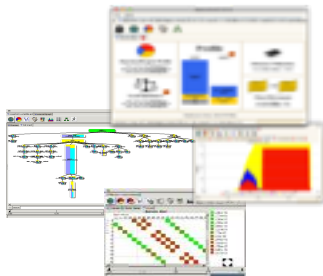
This simple change improved  
snswp3d by 50%

COMPUTE

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# Tips When Dealing with Big Applications

**Getting a Preview**



**Investigating Load imbalance**

**Speeding up Report Generation**

**Controlling Amount of Data**



# Perftool's Traditional Sampling Approach



- **Perftools profiles every MPI task on routine and line level**
- **In the resulting report**
  - Gives table of heavy hitters where the routine is evaluated on the average number of samples across all MPI tasks.
  - Gives load imbalance figure showing how minimum and maximum deviates from average
  - Typically does not show routines whose average is less than 1% of the total time
  - Sampling can not distinguish between MPI\_SYNC time; that is, the time waiting at the MPI function for all other MPI tasks to arrive and the actual MPI routine time. Therefore a lot of time for a MPI routine may be load imbalance



# Typical Profile at Scale

| Samp%  | Samp      | Imb.     | Imb.  | Group                      |
|--------|-----------|----------|-------|----------------------------|
|        |           | Samp     | Samp% | Function                   |
|        |           |          |       | PE=HIDE                    |
| 100.0% | 299,066.1 | --       | --    | Total                      |
| -----  |           |          |       |                            |
| 56.8%  | 169,977.1 | --       | --    | MPI                        |
| -----  |           |          |       |                            |
| 28.5%  | 85,307.3  | 37,316.7 | 30.5% | MPI_ALLREDUCE              |
| 26.6%  | 79,700.7  | 51,912.3 | 39.5% | mpi_waitall                |
| =====  |           |          |       |                            |
| 43.0%  | 128,473.8 | --       | --    | ETC                        |
| -----  |           |          |       |                            |
| 4.8%   | 14,233.0  | 1,410.0  | 9.0%  | routine1                   |
| 2.9%   | 8,607.9   | 11,569.1 | 57.4% | routine2                   |
| 2.6%   | 7,818.9   | 476.1    | 5.7%  | routine3                   |
| 2.4%   | 7,041.9   | 4,443.1  | 38.7% | routine4                   |
| 2.3%   | 6,911.4   | 771.6    | 10.1% | routine5                   |
| 2.1%   | 6,284.8   | 6,075.2  | 49.2% | __intel_mic_avx512f_memset |
| 2.1%   | 6,220.8   | 10,186.2 | 62.1% | routine6                   |
| 1.7%   | 4,992.0   | 2,480.0  | 33.2% | routine7                   |
| 1.4%   | 4,277.9   | 1,902.1  | 30.8% | routine8                   |
| 1.3%   | 3,869.4   | 294.6    | 7.1%  | routine9                   |
| 1.2%   | 3,583.1   | 5,093.9  | 58.7% | routine10                  |
| 1.0%   | 2,992.9   | 83.1     | 2.7%  | routine11                  |
| 1.0%   | 2,909.3   | 1,848.7  | 38.9% | routine12                  |

# Analysis of xRage at LANL



- This approach was taken on xRage running on over 256,000 MPI tasks
- A large amount of time  $> 75\%$  was attributed to MPI routines. Why? Was it load imbalance or actual time to do MPI operation?



# How to Find the Offending Moles

- **Ran both sampling and tracing experiments which generated tremendous amount of data**
  - The post processing step took longer than the computation
    - Choose subset of nodes to analyze
    - Needed tracing to identify where the MPI\_SYNC time occurred, giving us a clue to location of offending routine
    - Use pat\_regions to tunnel down to the offending code



# How to Reduce Performance Data

- **Choose subset of nodes**

- `user@login> export PAT_RT_EXPFFILE_PES=0,128,512`

- **Trace MPI routines to see if there is MPI\_SYNC time**

- `user@login> pat_build -g mpi ./my_program`

- **Use pat\_region API to drill down to finer granularity**

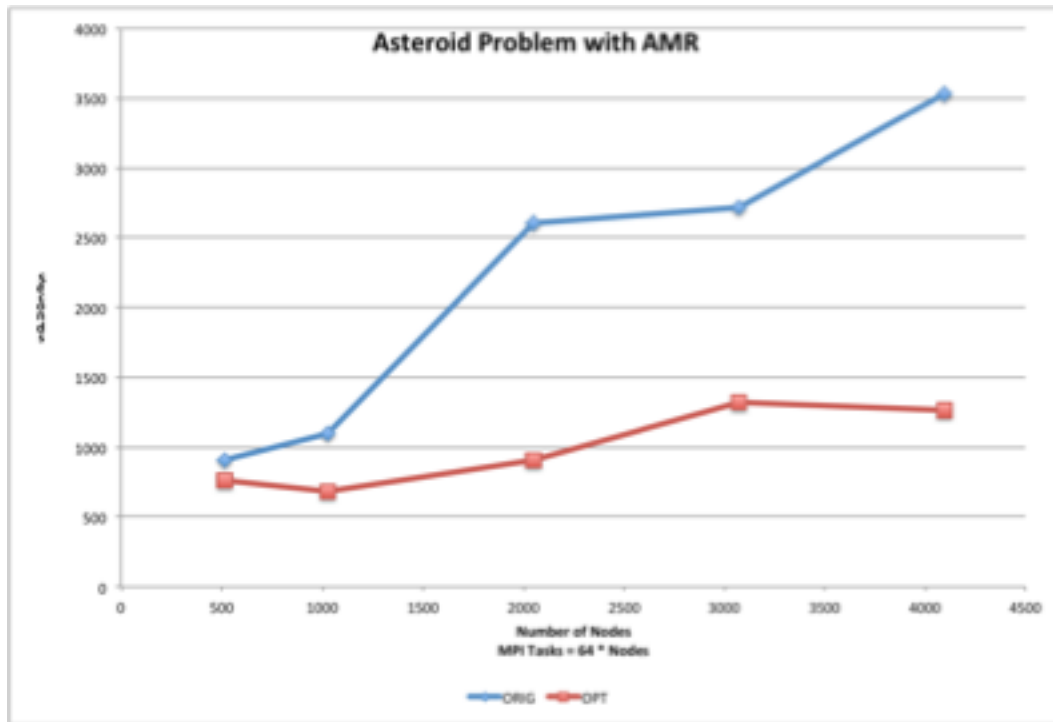
- See `pat_help` utility for API details
- Example: `user@login> pat_help regions C`

# And the results



- **Identified two separate areas that contributed to the load imbalance**
  - One was in the AMR section where each MPI task needed to figure out who was going to see them data
  - The other was in interpolating from one grid to another

# Significant Scalability Improvements in AMR via RMA Alltoall and Comm Caching



- The results are outstanding!
- ~3x performance improvement at scale
  - Total application runtime!
- RMA based Alltoall
- Caching and reuse of AMR communication pattern

# Leslie3D

The main purpose of this code is to model chemically reacting (i.e., burning) turbulent flows. Various different physical models are available in this algorithm but for this benchmark, only the basic conservation equations will be solved. Many, many different configurations can be modeled; however, for the sake of scalability and easy of use, only a rather simple configuration will be considered.



# Leslie3D

- MPI only
- Some vectorization

# Sampling Profile 64 MPI Tasks on 8 Nodes



|        |          |       |       |               |
|--------|----------|-------|-------|---------------|
| 100.0% | 21,119.9 | --    | --    | Total         |
| 94.1%  | 19,868.2 | --    | --    | USER          |
| 19.3%  | 4,083.9  | 117.1 | 2.8%  | visck_        |
| 18.3%  | 3,859.1  | 80.9  | 2.1%  | viscj_        |
| 18.0%  | 3,805.6  | 151.4 | 3.9%  | visci_        |
| 6.0%   | 1,273.0  | 82.0  | 6.1%  | fluxk_        |
| 5.1%   | 1,076.7  | 57.3  | 5.1%  | extrapk_      |
| 5.1%   | 1,075.2  | 84.8  | 7.4%  | fluxi_        |
| 5.1%   | 1,074.0  | 65.0  | 5.8%  | extrapi_      |
| 5.0%   | 1,050.8  | 65.2  | 5.9%  | fluxj_        |
| 4.3%   | 902.8    | 38.2  | 4.1%  | update_       |
| 4.1%   | 862.0    | 40.0  | 4.5%  | extrapj_      |
| 1.3%   | 278.9    | 77.1  | 22.0% | mpicx_        |
| 5.6%   | 1,178.1  | --    | --    | MPI           |
| 3.2%   | 676.2    | 312.8 | 32.1% | MPI_SEND      |
| 1.0%   | 209.6    | 64.4  | 23.9% | MPI_ALLREDUCE |



Three Moles



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# Call Tree with Loops



They are all called from high level loops

| Time%  | Time       | Calls       | Calltree             |
|--------|------------|-------------|----------------------|
|        |            |             | PE=HIDE              |
| 100.0% | 242.649260 | --          | Total                |
| -----  |            |             |                      |
| 100.0% | 242.649223 | 2.0         | les3d_               |
| 99.2%  | 240.654228 | --          | les3d_.LOOP.3.li.216 |
| -----  |            |             |                      |
| 97.9%  | 237.444979 | --          | les3d_.LOOP.4.li.272 |
| -----  |            |             |                      |
| 29.1%  | 70.519335  | 4,000.0     | fluxk_               |
| -----  |            |             |                      |
| 17.7%  | 42.941276  | --          | fluxk_.LOOP.1.li.28  |
|        |            |             | fluxk_.LOOP.2.li.29  |
| 17.7%  | 42.941276  | 9,408,000.0 | visck_               |
| 6.6%   | 16.130702  | 4,000.0     | fluxk_(exclusive)    |
| 4.7%   | 11.447357  | 4,000.0     | extrapk_             |
| =====  |            |             |                      |
| 28.1%  | 68.288330  | 4,000.0     | fluxj_               |
| -----  |            |             |                      |
| 18.3%  | 44.519098  | --          | fluxj_.LOOP.1.li.28  |
|        |            |             | fluxj_.LOOP.2.li.29  |
| 18.3%  | 44.519098  | 9,408,000.0 | viscj_               |
| 5.8%   | 14.084979  | 4,000.0     | fluxj_(exclusive)    |
| 4.0%   | 9.684254   | 4,000.0     | extrapj_             |
| =====  |            |             |                      |

| Time% | Time      | Calls        | Calltree               |
|-------|-----------|--------------|------------------------|
|       |           |              | PE=HIDE                |
| 27.2% | 65.960873 | 4,000.0      | fluxi_                 |
| ----- |           |              |                        |
| 15.0% | 36.464645 | --           | fluxi_.LOOP.1.li.21    |
|       |           |              | fluxi_.LOOP.2.li.22    |
| 15.0% | 36.464645 | 9,216,000.0  | visci_                 |
| 6.3%  | 15.328236 | 4,000.0      | extrapi_               |
| ----- |           |              |                        |
| 3.5%  | 8.424708  | 4,000.0      | extrapi_(exclusive)    |
| 2.8%  | 6.903528  | --           | extrapi_.LOOP.1.li.128 |
|       |           |              | extrapi_.LOOP.2.li.129 |
| 2.8%  | 6.903528  | 10,609,000.0 | exi4_                  |
| ===== |           |              |                        |
| 5.8%  | 14.167993 | 4,000.0      | fluxi_(exclusive)      |
| ===== |           |              |                        |
| 9.6%  | 23.356145 | 4,000.0      | parallel_              |
| ----- |           |              |                        |
| 7.2%  | 17.457089 | --           | parallel_.LOOP.1.li.16 |
| 7.2%  | 17.457089 | 20,000.0     | mpicx_                 |
| 2.4%  | 5.843909  | 20,000.0     | ghost_                 |
| ===== |           |              |                        |
| 3.6%  | 8.788456  | 4,000.0      | update_                |
| ===== |           |              |                        |
| 1.1%  | 2.557943  | 401.0        | tmstep_                |
| ===== |           |              |                        |

# Do Loop Table

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

| Loop<br>Incl<br>Time% | Loop Incl<br>Time | Loop Hit  | Loop<br>Trips<br>Avg | Loop<br>Trips<br>Min | Loop<br>Trips<br>Max | Function=/.LOOP[.]<br>PE=HIDE |
|-----------------------|-------------------|-----------|----------------------|----------------------|----------------------|-------------------------------|
| -----                 |                   |           |                      |                      |                      |                               |
| 99.2%                 | 246.816563        | 1         | 2,000.0              | 2,000                | 2,000                | les3d_.LOOP.3.li.216          |
| 97.9%                 | 243.603685        | 2,000     | 2.0                  | 2                    | 2                    | les3d_.LOOP.4.li.272          |
| 24.3%                 | 60.541874         | 4,000     | 48.0                 | 48                   | 48                   | fluxk_.LOOP.1.li.28           |
| 24.1%                 | 60.069820         | 4,000     | 48.0                 | 48                   | 48                   | fluxj_.LOOP.1.li.28           |
| 22.9%                 | 57.005766         | 192,000   | 49.0                 | 49                   | 49                   | fluxj_.LOOP.2.li.29           |
| 22.4%                 | 55.615468         | 192,000   | 49.0                 | 49                   | 49                   | fluxk_.LOOP.2.li.29           |
| 20.9%                 | 52.076589         | 4,000     | 48.0                 | 48                   | 48                   | fluxi_.LOOP.1.li.21           |
| 20.9%                 | 52.070251         | 192,000   | 48.0                 | 48                   | 48                   | fluxi_.LOOP.2.li.22           |
| 17.1%                 | 42.629610         | 9,408,000 | 48.0                 | 48                   | 48                   | viscj_.LOOP.1.li.340          |
| 16.5%                 | 40.972257         | 9,408,000 | 48.0                 | 48                   | 48                   | visck_.LOOP.1.li.344          |
| 13.9%                 | 34.612953         | 9,216,000 | 49.0                 | 49                   | 49                   | visci_.LOOP.1.li.782          |
| 7.0%                  | 17.507682         | 4,002     | 5.0                  | 5                    | 5                    | parallel_.LOOP.1.li.16        |
| 5.0%                  | 12.451170         | 4,000     | 51.5                 | 51                   | 52                   | extrapi_.LOOP.1.li.128        |
| 5.0%                  | 12.448703         | 206,000   | 51.5                 | 51                   | 52                   | extrapi_.LOOP.2.li.129        |
| 4.6%                  | 11.434859         | 4,000     | 49.0                 | 49                   | 49                   | extrapk_.LOOP.1.li.138        |
| 4.6%                  | 11.432312         | 196,000   | 51.5                 | 51                   | 52                   | extrapk_.LOOP.2.li.140        |
| 3.9%                  | 9.672461          | 4,000     | 51.5                 | 51                   | 52                   | extrapj_.LOOP.1.li.135        |
| 3.9%                  | 9.668853          | 206,000   | 49.0                 | 49                   | 49                   | extrapj_.LOOP.2.li.136        |

Mesh Loops of  
Reasonable  
Length

# Look at Threading Using OpenMP

- **First examine the loops in FLUX routines using Reveal**
  - Create program library `-hwp -hpl=leslie.pl` at build time
  - Gather DO loop statistics with `perftools-lite-loops`
  - `user@login> reveal my_program library my_perftools statistics`
    - Select one of the three high level loops in `fluxk`, `flukj`, `fluxi`

# Reveal Example Scoping Results



Loops with scoping information are flagged. Red needs user assistance

Source - /home/users/hedineval/shone...  
do i = 1, 100  
radius = zrc(sweep\*isz)  
theta = zrc(j\*sweep\*js)  
stheta = sin(theta)  
radius = radius \* stheta  
! Put state variables into 3D arrays, padding with 6 ghost zones  
do k = 1, rped  
do k = 1, ks  
x = k + ks\*(k-1) + 6  
r(n) = recv3(1, j, k, i, n)  
g(n) = recv3(2, j, k, i, n)  
u(n) = recv3(5, j, k, i, n)  
v(n) = recv3(3, j, k, i, n)  
w(n) = recv3(4, j, k, i, n)

Auto: Line 51  
● A loop starting at line 51 was scoped with errors. See Scoping Tool for more information.  
● "ppm" (called from "sweep") was not inlined because "iD" was detected in "volume".  
● "ppm" (called from "sweep") was not inlined because the enclosing loop body did not completely flatten.  
● A loop starting at line 105 is flat (contains no external calls).  
● A loop starting at line 105 was not vectorized because it does not map well onto the target architecture.  
● A loop starting at line 105 was unrolled 8 times.  
● A loop starting at line 51 was not vectorized because it contains a call to subroutine "ppm" on line 81.  
● A loop starting at line 52 was not vectorized because it contains a call to subroutine "ppm" on line 81.  
● A loop starting at line 59 is flat (contains no external calls).  
● A loop starting at line 59 was not vectorized because a better candidate was found at line 60.  
● A loop starting at line 60 is flat (contains no external calls).  
● A loop starting at line 60 was not vectorized because it does not map well onto the target architecture.  
● A loop starting at line 60 was unrolled 8 times.  
● A loop starting at line 71 is flat (contains no external calls).  
● A loop starting at line 71 was vectorized.

Scope Loops | Scoping Results | sweep.F90: Loop @51

Call to iD at line 81 of sweep.F90  
4 /home/users/hedineval/shone... 190 34  
1 /home/users/hedineval/shone... 190 21  
2 /home/users/hedineval/shone... 190 73  
1 /home/users/hedineval/shone... 190 81  
Call to iD at line 81 of sweep.F90

| Name       | Type   | Scope      | Info                                                       |
|------------|--------|------------|------------------------------------------------------------|
| widremap_1 | Scalar | Unresolved | FAIL Possible recurrence involving this object.            |
| ks         | Array  | Unresolved | FAIL Possible resolvable recurrence involving this object. |
| ks         | Array  | Unresolved | FAIL Possible resolvable recurrence involving this object. |
| ks         | Array  | Unresolved | FAIL Possible resolvable recurrence involving this object. |
| ks         | Array  | Unresolved | WARN LastPrivate of array may be very expensive.           |
| ks         | Array  | Unresolved | FAIL Possible recurrence involving this object.            |
| ks         | Array  | Unresolved | FAIL Possible resolvable recurrence involving this object. |
| ks         | Array  | Unresolved | WARN LastPrivate of array may be very expensive.           |
| i          | Scalar | Private    |                                                            |
| j          | Scalar | Private    |                                                            |
| k          | Scalar | Private    |                                                            |
| n          | Scalar | Private    |                                                            |
| stheta     | Scalar | Private    |                                                            |
| theta      | Scalar | Private    |                                                            |
| gamma      | Scalar | Shared     |                                                            |
| isz        | Scalar | Shared     |                                                            |
| js         | Scalar | Shared     |                                                            |
| ks         | Scalar | Shared     |                                                            |
| ppm        | Scalar | Shared     |                                                            |

Find Name:

Insert Directive Show Directive Close

Parallelization inhibitor messages are provided to assist user with analysis

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# CCE Listing: FLUXI.lst (-h list=a)

```
19.  +                      CALL EXTRAPI ( FSI )
20.                      ! Directive inserted by Cray Reveal.  May be incomplete.
21.  M-----< !$OMP parallel do default(none)
22.  M          !$OMP& private (i,j,k,l,qs,qsp,qspi)
23.  M          !$OMP& shared (dq,dtv,iadd,icmax,jcmax,kcmax,pav,qav,six,siy,siz,u,
24.  M          !$OMP&          uav,v,vav,w,wav)
25.  M          !$OMP& firstprivate(fsi)
26.  + M m-----<          DO K = 1, KCMAX
27.  + M m 3-----<          DO J = 1, JCMAX
28.  M m 3
29.  M m 3 fV-----<>          QS(0:ICMAX) = UAV(0:ICMAX,J,K) * SIX(0:ICMAX,J,K) +
30.  M m 3          >          VAV(0:ICMAX,J,K) * SIY(0:ICMAX,J,K) +
31.  M m 3          >          WAV(0:ICMAX,J,K) * SIZ(0:ICMAX,J,K)
32.  M m 3
```

Reveal did not auto-magically do this. It pointed out several unresolved variables. In this case, the user had to scope the questionable variable as private or shared.

# FLUXI.lst (1 of 2)

```
19.  +                CALL EXTRAPI ( FSI )
20.                ! Directive inserted by Cray Reveal.  May be incomplete.
21.  M-----< !OMP parallel do default(none)
22.  M          !OMP& private (i,j,k,l,qs,qsp,qspi)
23.  M          !OMP& shared (dq,dtv,iadd,icmax,jcmax,kcmax,pav,qav,six,siy,siz,u,
24.  M          !OMP&          uav,v,vav,w,wav)
25.  M          !OMP& firstprivate(fsi)
26.  + M m-----< DO K = 1, KCMAX
27.  + M m 3-----< DO J = 1, JCMAX
28.  M m 3
29.  M m 3 fV-----<> QS(0:ICMAX) = UAV(0:ICMAX,J,K) * SIX(0:ICMAX,J,K)
30.  M m 3 > VAV(0:ICMAX,J,K) * SIY(0:ICMAX,J,K) +
31.  M m 3 > WAV(0:ICMAX,J,K) * SIZ(0:ICMAX,J,K)
32.  M m 3
33.  M m 3 IF ( NSCHEME .EQ. 2 ) THEN
34.  M m 3 D-----< DO I = 0, ICMAX
35.  M m 3 D L = I + 1 - IADD
36.  M m 3 D QSP = U(L,J,K) * SIX(I,J,K)
37.  M m 3 D > V(L,J,K) * SIY(I,J,K) +
38.  M m 3 D > W(L,J,K) * SIZ(I,J,K)
39.  M m 3 D QSPI = (QSP - QS(I)) * DBLE(1 - 2 * QS(I)) + QSP
40.  M m 3 D IF ( QSPI .GT. 0.0D0 ) QS(I) = 0.5D0 * (QS(I) + QSPI)
41.  M m 3 D-----> ENDDO
42.  M m 3 ENDIF
43.  M m 3
```

Array syntax –  
vectorized and  
fused with other  
loops

Compiler knows  
NSCHEME is  
not equal to 2



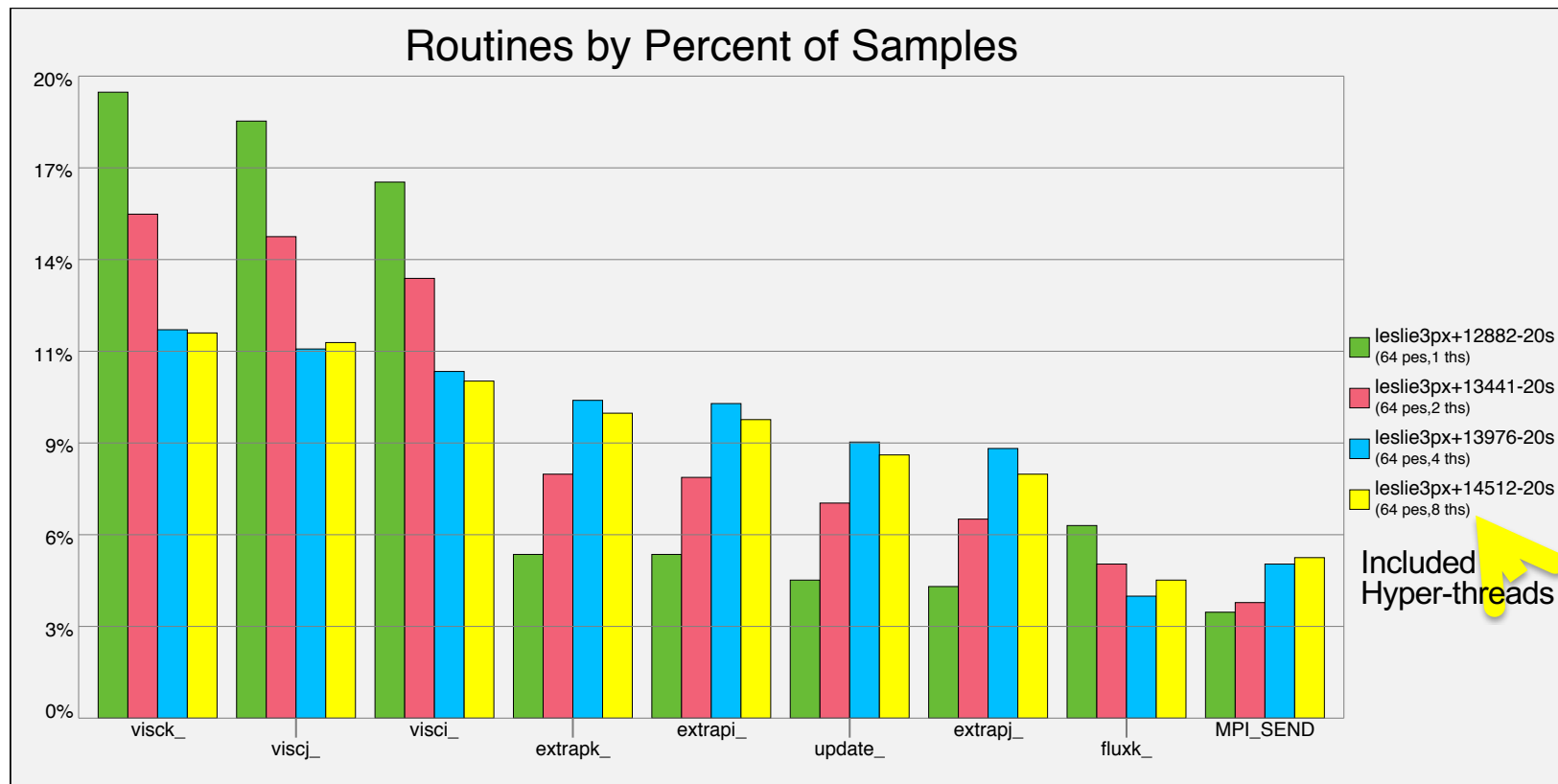
# FLUXI.lst (2 of 2)



```
44.      M m 3 f-----<>      FSI(0:ICMAX,1) = QAV(0:ICMAX,J,K,1) * QS(0:ICMAX)
45.      M m 3 f-----<>      FSI(0:ICMAX,2) = QAV(0:ICMAX,J,K,2) * QS(0:ICMAX) +
46.      M m 3                                     >      PAV(0:ICMAX,J,K) * SIX(0:ICMAX,J,K)
47.      M m 3 f-----<>      FSI(0:ICMAX,3) = QAV(0:ICMAX,J,K,3) * QS(0:ICMAX) +
48.      M m 3                                     >      PAV(0:ICMAX,J,K) * SIY(0:ICMAX,J,K)
49.      M m 3 fVr2-----<>      FSI(0:ICMAX,4) = QAV(0:ICMAX,J,K,4) * QS(0:ICMAX) +
50.      M m 3                                     >      PAV(0:ICMAX,J,K) * SIZ(0:ICMAX,J,K)
51.      M m 3 f-----<>      FSI(0:ICMAX,5) = (QAV(0:ICMAX,J,K,5) + PAV(0:ICMAX,J,K)) *
52.      M m 3                                     >      QS(0:ICMAX)
53.      M m 3
54.      M m 3      IF ( ISGSK .EQ. 1 ) THEN
55.      M m 3          FSI(0:ICMAX,7) = QAV(0:ICMAX,J,K,7)
56.      M m 3      ENDIF
57.      M m 3
58.      M m 3      IF ( ICHEM .GT. 0 ) THEN
59.      M m 3 D-----<      DO L = 8, 7 + NSPECI
60.      M m 3 D          FSI(0:ICMAX,L) = QAV(0:ICMAX,J,K,L) * QS(0:ICMAX)
61.      M m 3 D----->      ENDDO
62.      M m 3      ENDIF
63.      M m 3
64.      + M m 3      IF ( VISCOUS ) CALL VISCI ( 0, ICMAX, J, K, FSI )
65.      M m 3
```

VISCI is called  
from OpenMP loop

# 64 MPI Tasks on 8 Nodes



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# Observations From Timings

- **VISC(I,J,K) still using significant amount of time**
- **EXTRAP(I,J,K) needs to be addressed**
- **UPDATE needs to be addressed**

# Concern with the VISCs



```
ftn-6383 ftn: VECTOR VISCK, File = fluxk.f, Line = 344
```

A loop starting at line 344 requires an estimated 25 vector registers at line 485; 2 of these have been preemptively forced to memory.

```
ftn-6204 ftn: VECTOR VISCK, File = fluxk.f, Line = 344
```

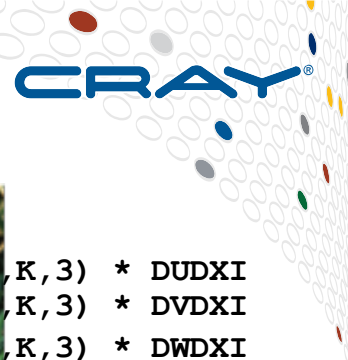
A loop starting at line 344 was vectorized.

# Modifications



- **Optimization: promoted 12 scalars to arrays to enable the lengthy loop to be split into three separate loops**
- **Result: all three routines improved by 25%**

# Modifications (continued)



```

<      DUDX = T11(I,J,K,3) * DUDXI
<      DVDX = T11(I,J,K,3) * DVDXI
<      DWDX = T11(I,J,K,3) * DWDXI
<      DTDX = T11(I,J,K,3) * DTDXI
<
<      DUDY = T21(I,J,K,3) * DUDXI
<      DVDY = T21(I,J,K,3) * DVDXI
<      DWDY = T21(I,J,K,3) * DWDXI
<      DTDY = T21(I,J,K,3) * DTDXI
<
<      DUDZ = T31(I,J,K,3) * DUDXI
<      DVDZ = T31(I,J,K,3) * DVDXI
<      DWDZ = T31(I,J,K,3) * DWDXI
<      DTDZ = T31(I,J,K,3) * DTDXI
<
    
```

**A**



```

--      DUDX = T11(I,J,K,3) * DUDXI
>      DVDX = T11(I,J,K,3) * DVDXI
>      DWDX = T11(I,J,K,3) * DWDXI
>      DTDX = T11(I,J,K,3) * DTDXI
>
>      DUDY(I) = T21(I,J,K,3) * DUDXI
>      DVDY(I) = T21(I,J,K,3) * DVDXI
>      DWDY(I) = T21(I,J,K,3) * DWDXI
>      DTDY(I) = T21(I,J,K,3) * DTDXI
>
>      DUDZ(I) = T31(I,J,K,3) * DUDXI
>      DVDZ(I) = T31(I,J,K,3) * DVDXI
>      DWDZ(I) = T31(I,J,K,3) * DWDXI
>      DTDZ(I) = T31(I,J,K,3) * DTDXI
    
```

**Whacked**

# Reveal Scoping of EXTRAP Routines

```

142.
143.                                ! Directive inserted by Cray Reveal.  May be incomplete.
144.      M-----< !$OMP parallel do default(none)
145.      M                                !$OMP&  private (rwrk,j,k,kg)
146.      M                                !$OMP&  shared  (i1,i2,j1,j2,kcmax,kmax,kstart,pav,qav,tav,
147.      M                                !$OMP&                                uav,vav,wav)
148.  + M m-----<      DO K = 0, KCMAX
149.      M m                                KG = K + KSTART - 1
150.  + M m 3-----<      DO J = J1, J2
151.      M m 3
152.      M m 3                                IF ( NSCHEME .EQ. 2 .OR. (.NOT. KPERIODIC .AND.
153.      M m 3                                >                                (KG .EQ. 0 .OR. KG .EQ. KMAX-1))) THEN
154.  + M m 3                                CALL EXK2 ( I1, I2, J, K )
155.      M m 3                                ELSE
156.  + M m 3                                CALL EXK4 ( I1, I2, J, K,
157.      M m 3                                >                                RWRK(I1,1) , RWRK(I1,2) , RWRK(I1,3) )
158.      M m 3                                ENDIF

```

Once again Reveal needed help scoping some of the arrays that had questionable usage

# Reveal Scoping of UPDATE Routine

```
9.          ! Directive inserted by Cray Reveal.  May be incomplete.
10.  M-----< !$OMP parallel do default(none)
11.  M          !$OMP& private (i,j,k,ke)
12.  M          !$OMP& shared (dq,icmax,jcmax,kcmax,m,n,p,q,t,u,v,w)
13.  + M m-----<      DO K = 1, KCMAX
14.  + M m 3-----<      DO J = 1, JCMAX
15.  M m 3 V--<          DO I = 1, ICMAX
16.  M m 3 V
17.  M m 3 V          IF ( N .EQ. 1 ) THEN
18.  M m 3 V              Q(I,J,K,1,M) = Q(I,J,K,1,N) + DQ(I,J,K,1)
19.  M m 3 V              Q(I,J,K,2,M) = Q(I,J,K,2,N) + DQ(I,J,K,2)
20.  M m 3 V              Q(I,J,K,3,M) = Q(I,J,K,3,N) + DQ(I,J,K,3)
21.  M m 3 V              Q(I,J,K,4,M) = Q(I,J,K,4,N) + DQ(I,J,K,4)
22.  M m 3 V              Q(I,J,K,5,M) = Q(I,J,K,5,N) + DQ(I,J,K,5)
23.  M m 3 V          ELSE
24.  M m 3 V              Q(I,J,K,1,M) = 0.5D+00 * (Q(I,J,K,1,M) +
25.  M m 3 V                  >              Q(I,J,K,1,N) + DQ(I,J,K,1))
26.  M m 3 V              Q(I,J,K,2,M) = 0.5D+00 * (Q(I,J,K,2,M) +
27.  M m 3 V                  >              Q(I,J,K,2,N) + DQ(I,J,K,2))
28.  M m 3 V              Q(I,J,K,3,M) = 0.5D+00 * (Q(I,J,K,3,M) +
```

This one Reveal did  
without help







# Another Modification to UPDATE

```
10.  + 1-----<          DO K = 1, KCMAX
11.  + 1 2-----<          DO J = 1, JCMAX
12.    1 2 iVbr4-----<          DO I = 1, ICMAX
13.      1 2 iVbr4
14.      1 2 iVbr4          IF ( N .EQ. 1 ) THEN
15.  + 1 2 iVbr4 ib--<>      Q(I,J,K,1:5,M) = Q(I,J,K,1:5)
16.      1 2 iVbr4          ELSE
17.  + 1 2 iVbr4 ib--<>      Q(I,J,K,1:5,M) = Q(I,J,K,1:5,M) +
18.      1 2 iVbr4          Q(I,J,K,1:5,N) + DQ(I,J,K,1:5)
19.      1 2 iVbr4          >
20.      1 2 iVbr4          >
21.      1 2 iVbr4          U(I,J,K) = Q(I,J,K,2,M) / Q(I,J,K,1,M)
22.      1 2 iVbr4          V(I,J,K) = Q(I,J,K,3,M) / Q(I,J,K,1,M)
23.      1 2 iVbr4          W(I,J,K) = Q(I,J,K,4,M) / Q(I,J,K,1,M)
24.      1 2 iVbr4
25.      1 2 iVbr4          KE = 0.5D+00 * (U(I,J,K) * U(I,J,K) +
26.      1 2 iVbr4          V(I,J,K) * V(I,J,K) +
27.      1 2 iVbr4          W(I,J,K) * W(I,J,K))
28.      1 2 iVbr4
29.      1 2 iVbr4          T(I,J,K) = (Q(I,J,K,5,M) / Q(I,J,K,1,M) - KE) / CVAIR
30.      1 2 iVbr4          P(I,J,K) = Q(I,J,K,1,M) * RGAIR * T(I,J,K)
31.      1 2 iVbr4----->          ENDDO
32.      1 2----->          ENDDO
33.      1----->          ENDDO
```



# Another Modification to UPDATE



15c18,22

```
< Q(I,J,K,1:5,M) = Q(I,J,K,1:5,N) + DQ(I,J,K,1:5,M)
```

---

```
> Q(I,J,K,1,M) = Q(I,J,K,1,N) + DQ(I,J,K,1,M)
> Q(I,J,K,2,M) = Q(I,J,K,2,N) + DQ(I,J,K,2,M)
> Q(I,J,K,3,M) = Q(I,J,K,3,N) + DQ(I,J,K,3,M)
> Q(I,J,K,4,M) = Q(I,J,K,4,N) + DQ(I,J,K,4,M)
> Q(I,J,K,5,M) = Q(I,J,K,5,N) + DQ(I,J,K,5,M)
```



17,18c24,33

```
< Q(I,J,K,1:5,M) = 0.5D+00 * (Q(I,J,K,1:5,M) +
< > Q(I,J,K,1:5,N) + DQ(I,J,K,1:5,M))
```

---

```
> Q(I,J,K,1,M) = 0.5D+00 * (Q(I,J,K,1,M) +
> > Q(I,J,K,1,N) + DQ(I,J,K,1,M))
> Q(I,J,K,2,M) = 0.5D+00 * (Q(I,J,K,2,M) +
> > Q(I,J,K,2,N) + DQ(I,J,K,2,M))
> Q(I,J,K,3,M) = 0.5D+00 * (Q(I,J,K,3,M) +
> > Q(I,J,K,3,N) + DQ(I,J,K,3,M))
> Q(I,J,K,4,M) = 0.5D+00 * (Q(I,J,K,4,M) +
> > Q(I,J,K,4,N) + DQ(I,J,K,4,M))
> Q(I,J,K,5,M) = 0.5D+00 * (Q(I,J,K,5,M) +
> > Q(I,J,K,5,N) + DQ(I,J,K,5,M))
```

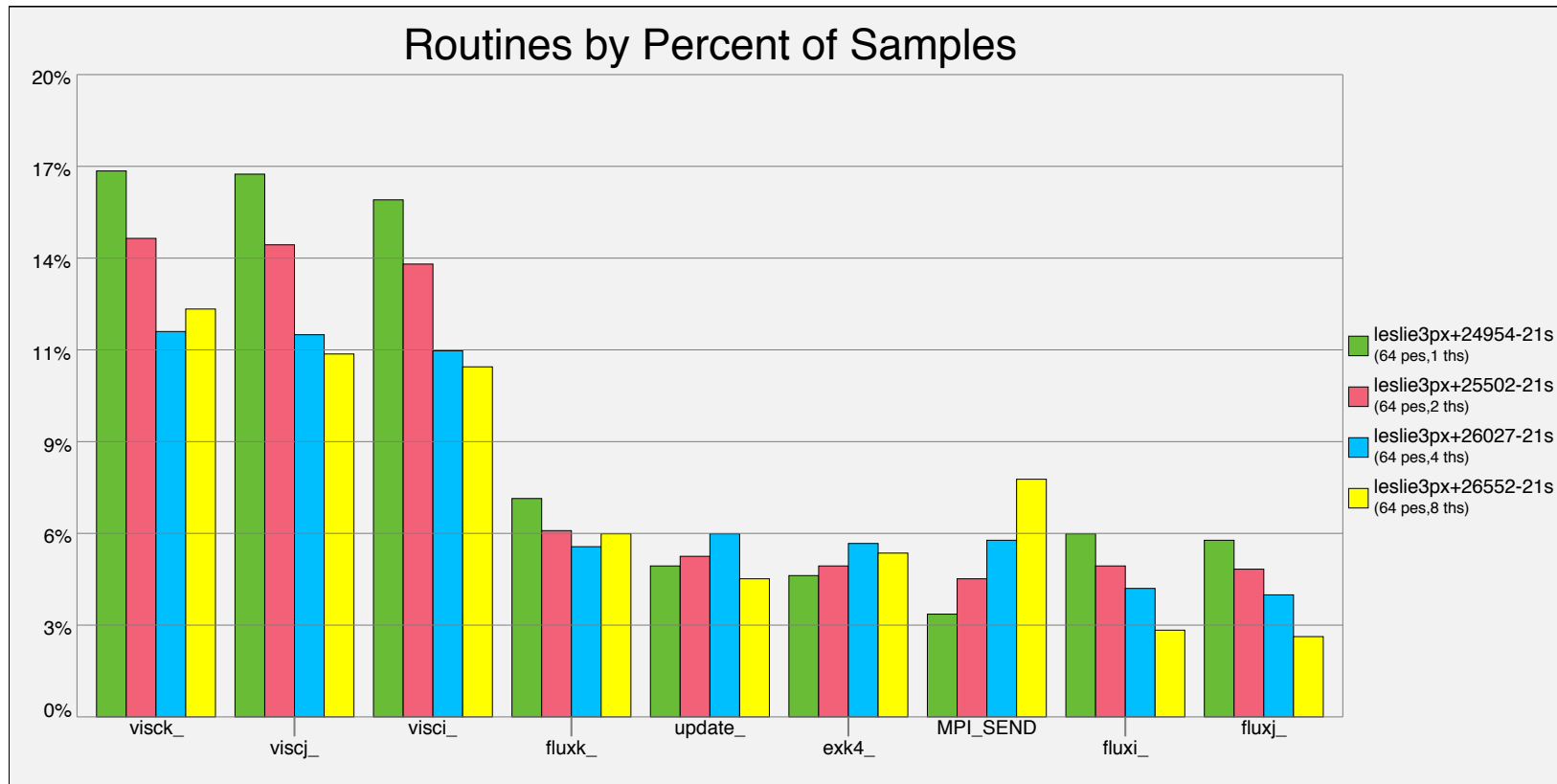
# Whacked

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# Optimization Results for 64 MPI Tasks on 8 Nodes



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# Final Sampling Profile



Table 1: Profile by Function

| Samp%  | Samp    | Imb.  | Imb.  | Group                                      |
|--------|---------|-------|-------|--------------------------------------------|
|        |         | Samp  | Samp% | Function=[MAX10]<br>PE=HIDE<br>Thread=HIDE |
| 100.0% | 9,268.0 | --    | --    | Total                                      |
| 86.4%  | 8,003.3 | --    | --    | USER                                       |
| 12.0%  | 1,114.2 | 84.8  | 7.2%  | visck_                                     |
| 11.9%  | 1,106.2 | 58.8  | 5.1%  | viscj_                                     |
| 11.4%  | 1,054.9 | 49.1  | 4.5%  | visci_                                     |
| 5.7%   | 531.1   | 46.9  | 8.2%  | update_                                    |
| 5.4%   | 499.0   | 45.0  | 8.4%  | exk4_                                      |
| 5.3%   | 490.8   | 65.2  | 11.9% | fluxk_                                     |
| 5.2%   | 484.0   | 41.0  | 7.9%  | extrapi_                                   |
| 4.6%   | 424.7   | 35.3  | 7.8%  | exi4_                                      |
| 4.1%   | 382.4   | 50.6  | 11.9% | exj4_                                      |
| 11.6%  | 1,078.5 | --    | --    | MPI                                        |
| 5.5%   | 507.0   | 205.0 | 29.3% | MPI_SEND                                   |
| 1.9%   | 178.7   | --    | --    | ETC                                        |

**Best time on 8 nodes is with  
64 MPI tasks and 4 Threads  
per MPI task**

**2.3 times faster than original!**

# Pure MPI Profile

ORIGINAL

CRAY®

Table 1: Profile by Function

| Samp%  | Samp    | Imb. | Imb.  | Group               |
|--------|---------|------|-------|---------------------|
|        |         | Samp | Samp% | Function<br>PE=HIDE |
| 100.0% | 8,919.6 | --   | --    | Total               |
| 84.4%  | 7,532.4 | --   | --    | USER                |
| 12.4%  | 1,108.2 | 56.8 | 4.9%  | viscj_              |
| 11.8%  | 1,048.1 | 93.9 | 8.3%  | visci_              |
| 11.7%  | 1,047.8 | 74.2 | 6.6%  | visck_              |
| 6.0%   | 530.9   | 37.1 | 6.6%  | update_             |
| 5.8%   | 518.4   | 49.6 | 8.8%  | exk4_               |
| 5.8%   | 513.7   | 36.3 | 6.6%  | exi4_               |
| 4.9%   | 439.1   | 53.9 | 11.0% | exj4_               |
| 4.4%   | 392.1   | 41.9 | 9.7%  | fluxk_              |
| 4.3%   | 382.1   | 53.9 | 12.4% | fluxi_              |
| 4.2%   | 373.2   | 42.8 | 10.3% | fluxj_              |
| 4.0%   | 359.9   | 61.1 | 14.6% | extrapi_            |
| 2.1%   | 184.0   | 35.0 | 16.0% | extrapj_            |
| 1.8%   | 159.8   | 39.2 | 19.8% | extrapk_            |
| 1.4%   | 129.1   | 67.9 | 34.6% | mpicx_              |
| 1.4%   | 120.8   | 46.2 | 27.8% | parallel_           |
| 1.3%   | 114.9   | 57.1 | 33.3% | ghost_              |

Table 1: Profile by Function

| Samp%  | Samp    | Imb.  | Imb.  | Group               |
|--------|---------|-------|-------|---------------------|
|        |         | Samp  | Samp% | Function<br>PE=HIDE |
| 100.0% | 9,206.9 | --    | --    | Total               |
| 85.8%  | 7,899.0 | --    | --    | USER                |
| 18.1%  | 1,662.2 | 90.8  | 5.2%  | fluxj_              |
| 17.4%  | 1,602.9 | 225.1 | 12.4% | fluxk_              |
| 16.8%  | 1,542.4 | 109.6 | 6.7%  | fluxi_              |
| 9.3%   | 855.7   | 72.3  | 7.8%  | extrapi_            |
| 7.1%   | 652.3   | 53.7  | 7.6%  | extrapk_            |
| 6.5%   | 602.6   | 62.4  | 9.4%  | extrapj_            |
| 5.7%   | 528.0   | 60.0  | 10.2% | update_             |
| 1.4%   | 130.4   | 43.6  | 25.1% | mpicx_              |
| 1.3%   | 123.0   | 70.0  | 36.4% | parallel_           |
| 1.1%   | 100.7   | 81.3  | 44.8% | ghost_              |
| 13.7%  | 1,263.9 | --    | --    | MPI                 |
| 8.1%   | 749.8   | 270.2 | 26.6% | MPI_SEND            |
| 2.3%   | 209.7   | 101.3 | 32.7% | MPI_ALLREDUCE       |
| 1.5%   | 136.1   | 269.9 | 66.7% | MPI_WAIT            |
| 1.5%   | 135.8   | 119.2 | 46.9% | MPI_REDUCE          |

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# All That Work for Nothing?



- We could do a lot more to optimize for cache in the VISC(I,J,K) routines
- But, a pure MPI solution runs pretty well on multicore node like haswell, broadwell, skylake and even KNL

# Memory Analysis of the Optimized Code



Table 5: Profile by Group, Function, and Line

| Samp%  | Samp  | Imb. | Imb.  | MEM_LOAD_UOPS_RETIRED  | RESOURCE_STALLS       | Group                      |
|--------|-------|------|-------|------------------------|-----------------------|----------------------------|
|        |       | Samp | Samp% | :HIT_LFB:precise=2     | :ANY                  | Function=[MAX10]<br>Source |
|        |       |      |       |                        |                       | Line<br>PE=HIDE            |
| 100.0% | 359.1 | --   | --    | 37,453,764,107,885,936 | 586,696,060,451       | Total                      |
| 90.3%  | 324.2 | --   | --    | 33,675,842,152,965,068 | 538,408,160,657       | USER                       |
| 16.6%  | 59.7  | --   | --    | 6,020,925,677,307,978  | 98,381,410,309        | fluxk_                     |
| 3      |       |      |       |                        |                       | fluxk.f                    |
| 4      | 3.7%  | 13.4 | 9.6   | 42.2%                  | 1,411,772,930,846,618 | 22,424,492,033   line.36   |
| 4      | 1.1%  | 4.0  | 7.0   | 64.9%                  | 369,435,907,219,731   | 6,575,931,964   line.54    |
| 4      | 9.1%  | 32.6 | 37.4  | 54.3%                  | 3,294,136,838,755,624 | 53,681,888,808   line.76   |
| 14.7%  | 52.8  | --   | --    | 5,770,237,024,852,115  | 88,570,460,626        | visci_                     |
| 3      |       |      |       |                        |                       | fluxi.f                    |
| 4      | 1.1%  | 4.1  | 4.9   | 55.7%                  | 452,998,790,837,684   | 6,904,792,416   line.807   |
| 4      | 2.1%  | 7.5  | 9.5   | 57.0%                  | 818,036,651,385,400   | 12,609,245,898   line.822  |
| 13.8%  | 49.7  | --   | --    | 5,246,869,490,559,427  | 82,777,122,645        | fluxj_                     |
| 3      |       |      |       |                        |                       | fluxj.f                    |
| 4      | 2.8%  | 10.2 | 18.8  | 66.0%                  | 1,077,521,395,774,529 | 16,750,162,451   line.36   |
| 4      | 8.2%  | 29.3 | 40.7  | 59.0%                  | 3,118,214,977,991,204 | 48,910,720,877   line.76   |

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# Code in FLUXK Responsible for Memory Bandwidth Utilization



```
73.      M m
74. + M m ib-----<          DO K = 1, KCMAX
75. + M m ib i-----<          DO L = 1, 5
76.      M m ib i Vbr4--<>          DQ(1:IND,J,K,L) = DQ(1:IND
77.      M m ib i          >          DTV(1:IND,J,K) * (FSK
78.      M m ib i----->          ENDDO
79.      M m ib
80.      M m ib          IF (ISGSK .EQ. 1) THEN
81.      M m ib          DQ(1:IND,J,K,7) = DQ(1:IND,J,K,7) -
82.      M m ib          >          DTV(1:IND,J,K) * (FSK(1:IND,K,7) - FSK(1:IND,K-1,7))
83.      M m ib          ENDDIF
84.      M m ib
85.      M m ib          IF ( ICHM .GT. 0 ) THEN
86.      M m ib D-----<          DO L = 8, 7 + NSPECI
87.      M m ib D          DQ(1:IND,J,K,L) = DQ(1:IND,J,K,L) -
88.      M m ib D          >          DTV(1:IND,J,K) * (FSK(1:IND,K,L) - FSK(1:IND,K-1,L))
89.      M m ib D----->          ENDDO
90.      M m ib          ENDDIF
91.      M m ib
92.      M m ib----->          ENDDO
```





# Array Syntax and Automatic Blocking by the Compiler

A



by 33% -  
there is a lot  
X

```
73.      M m                      !dir$ noblocking
74. + M m 3-----<              DO K = 1, KCMAX
75.      M m 3 V-----<          DO I = 1, IND
76.      M m 3 V                      !dir$ unroll(5)
77.      M m 3 V w-----<        DO L = 1, 5
78.      M m 3 V w                      DQ(I,J,K,L) = DQ(I,J,K,L) -
79.      M m 3 V w                      >          DTV(I,J,K) * (FSK(I,K,L)
80.      M m 3 V w----->          ENDDO
81.      M m 3 V
82.      M m 3 V                      IF (ISGSK.EQ. 1) THEN
83.      M m 3 V                      DQ(I,J,K,7) = DQ(I,J,K,7) -
84.      M m 3 V                      >          DTV(I,J,K) * (FSK(I,K,7) - FSK(I,K-1,7))
85.      M m 3 V                      ENDIF
86.      M m 3 V
87.      M m 3 V                      IF ( ICHEM .GT. 0 ) THEN
88.      M m 3 V D-----<          DO L = 8, 7 + NSPECI
89.      M m 3 V D                      DQ(I,J,K,L) = DQ(I,J,K,L) -
90.      M m 3 V D                      >          DTV(I,J,K) * (FSK(I,K,L) - FSK(I,K-1,L))
91.      M m 3 V D----->          ENDDO
92.      M m 3 V                      ENDIF
93.      M m 3 V
94.      M m 3 V----->          ENDDO
95.      M m 3----->          ENDDO
96.      M m----->          ENDDO
```

Whacked



# VH1

---

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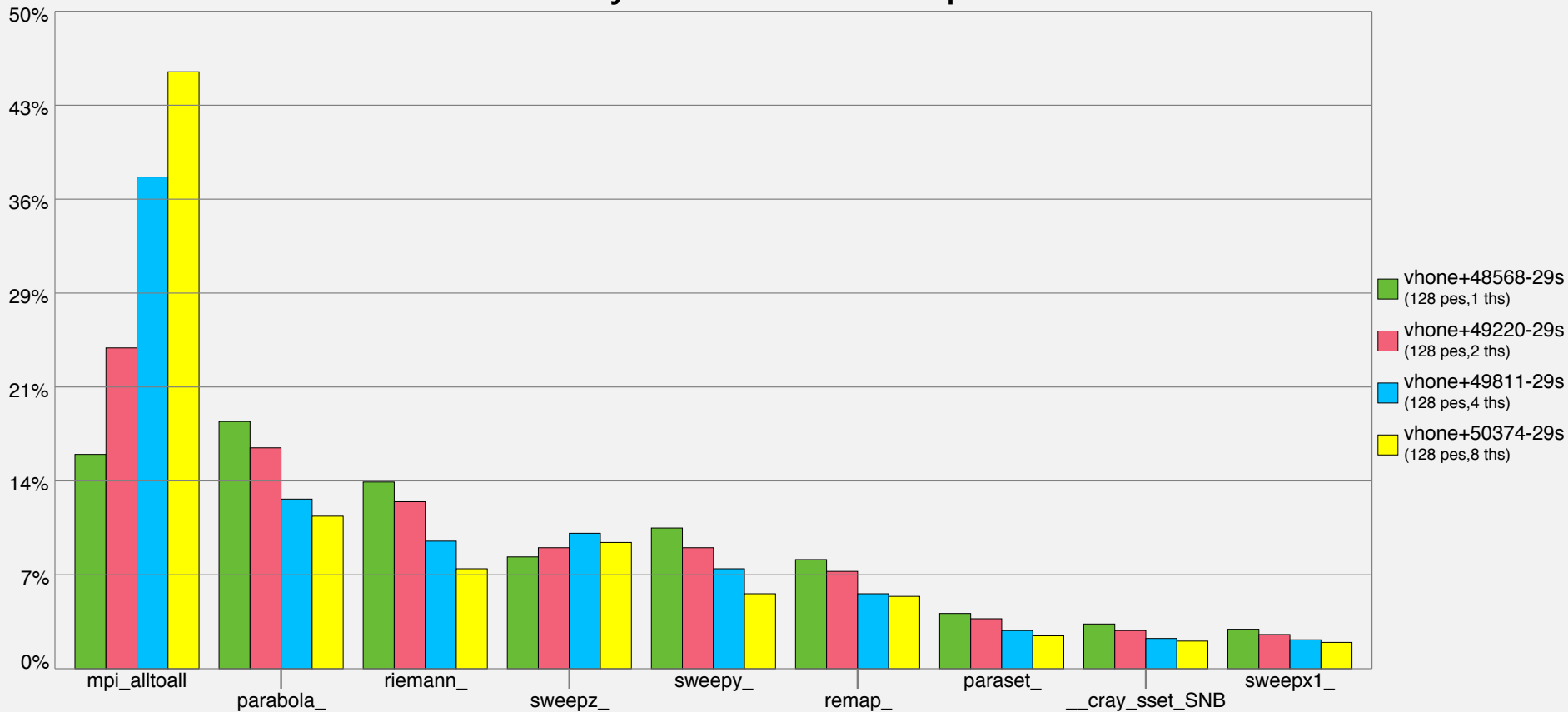
| ANALYZE

# VH1 Already Parallelized Using Reveal



- Need to investigate additional optimization
- Vectorization and Memory utilization optimization

# Routines by Percent of Samples



# Profile for 1 Thread and 4 Threads

Table 1: Profile by Function 1 Thread

| Samp%  | Samp     | Imb.  | Imb.  | Group                       |
|--------|----------|-------|-------|-----------------------------|
|        |          | Samp  | Samp% | Function=[MAX10]<br>PE=HIDE |
| 100.0% | 39,072.1 | --    | --    | Total                       |
| 77.5%  | 30,298.1 | --    | --    | USER                        |
| 18.8%  | 7,340.2  | 254.8 | 3.4%  | parabola_                   |
| 14.2%  | 5,533.8  | 362.2 | 6.2%  | riemann_                    |
| 10.7%  | 4,173.6  | 221.4 | 5.1%  | sweepy_                     |
| 8.5%   | 3,340.0  | 247.0 | 6.9%  | sweepz_                     |
| 8.3%   | 3,226.1  | 173.9 | 5.2%  | remap_                      |
| 4.2%   | 1,653.7  | 151.3 | 8.4%  | paraset_                    |
| 3.0%   | 1,184.3  | 76.7  | 6.1%  | sweepx1_                    |
| 2.9%   | 1,123.3  | 68.7  | 5.8%  | sweepx2_                    |
| 16.9%  | 6,600.0  | --    | --    | MPI                         |
| 16.3%  | 6,373.7  | 670.3 | 9.6%  | mpi_alltoall                |
| 5.5%   | 2,160.6  | --    | --    | ETC                         |
| 3.4%   | 1,328.0  | 110.0 | 7.7%  | __cray_sset_SNB             |

Table 1: Profile by Function 4 Threads

| Samp%  | Samp     | Imb.  | Imb.  | Group                                      |
|--------|----------|-------|-------|--------------------------------------------|
|        |          | Samp  | Samp% | Function=[MAX10]<br>PE=HIDE<br>Thread=HIDE |
| 100.0% | 16,290.4 | --    | --    | Total                                      |
| 58.4%  | 9,508.0  | --    | --    | USER                                       |
| 12.9%  | 2,105.5  | 167.5 | 7.4%  | parabola_                                  |
| 10.3%  | 1,679.0  | 107.0 | 6.0%  | sweepz_                                    |
| 9.7%   | 1,585.0  | 151.0 | 8.8%  | riemann_                                   |
| 7.6%   | 1,242.2  | 72.8  | 5.6%  | sweepy_                                    |
| 5.7%   | 926.7    | 77.3  | 7.8%  | remap_                                     |
| 2.9%   | 476.5    | 50.5  | 9.7%  | paraset_                                   |
| 2.2%   | 355.4    | 64.6  | 15.5% | sweepx1_                                   |
| 2.0%   | 323.2    | 33.8  | 9.5%  | sweepx2_                                   |
| 37.7%  | 6,135.4  | --    | --    | MPI                                        |
| 37.4%  | 6,095.4  | 100.6 | 1.6%  | mpi_alltoall                               |
| 3.8%   | 619.9    | --    | --    | ETC                                        |
| 2.3%   | 378.2    | 65.8  | 14.9% | __cray_sset_SNB                            |

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# Do Loop Table

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

| Loop<br>Incl<br>Time% | Loop Incl<br>Time | Loop Hit      | Loop<br>Trips<br>Avg | Loop<br>Trips<br>Min | Loop<br>Trips<br>Max | Function=/.LOOP[.]<br>PE=HIDE |
|-----------------------|-------------------|---------------|----------------------|----------------------|----------------------|-------------------------------|
| 100.0%                | 631.108612        | 1             | 50.0                 | 50                   | 50                   | vhone_.LOOP.2.li.205          |
| 30.6%                 | 193.127659        | 100           | 64.0                 | 64                   | 64                   | sweepy_.LOOP.1.li.38          |
| 30.6%                 | 193.127263        | 6,400         | 128.0                | 128                  | 128                  | sweepy_.LOOP.2.li.39          |
| 27.8%                 | 175.704223        | 50            | 128.0                | 128                  | 128                  | sweepz_.LOOP.05.li.53         |
| 27.8%                 | 175.703983        | 6,400         | 64.0                 | 64                   | 64                   | sweepz_.LOOP.06.li.54         |
| 20.6%                 | 130.290184        | 2,457,600     | 1,031.0              | 1,031                | 1,031                | riemann_.LOOP.2.li.63         |
| 14.0%                 | 88.344946         | 50            | 64.0                 | 64                   | 64                   | sweepx2_.LOOP.1.li.33         |
| 14.0%                 | 88.344688         | 3,200         | 128.0                | 128                  | 128                  | sweepx2_.LOOP.2.li.34         |
| 13.9%                 | 87.468636         | 50            | 64.0                 | 64                   | 64                   | sweepx1_.LOOP.1.li.33         |
| 13.9%                 | 87.468481         | 3,200         | 128.0                | 128                  | 128                  | sweepx1_.LOOP.2.li.34         |
| 10.3%                 | 64.960442         | 22,118,400    | 1,028.0              | 1,026                | 1,032                | parabola_.LOOP.7.li.75        |
| 5.6%                  | 35.320759         | 2,533,785,600 | 12.0                 | 12                   | 12                   | riemann_.LOOP.3.li.64         |
| 1.5%                  | 9.708508          | 409,600       | 16.0                 | 16                   | 16                   | sweepz_.LOOP.07.li.61         |
| 1.5%                  | 9.202399          | 50            | 128.0                | 128                  | 128                  | sweepz_.LOOP.01.li.22         |
| 1.5%                  | 9.201736          | 6,400         | 8.0                  | 8                    | 8                    | sweepz_.LOOP.02.li.23         |
| 1.5%                  | 9.198684          | 51,200        | 128.0                | 128                  | 128                  | sweepz_.LOOP.03.li.24         |
| 1.3%                  | 7.941815          | 50            | 64.0                 | 64                   | 64                   | sweepz_.LOOP.12.li.116        |
| 1.3%                  | 7.941276          | 3,200         | 64.0                 | 64                   | 64                   | sweepz_.LOOP.13.li.117        |
| 1.3%                  | 7.935293          | 204,800       | 16.0                 | 16                   | 16                   | sweepz_.LOOP.14.li.118        |

# Call Tree with Loops



Table 1: Function Calltree View

| Time%       | Time       | Calls       | Calltree              |
|-------------|------------|-------------|-----------------------|
|             |            |             | PE=HIDE               |
| 100.0%      | 623.115520 | --          | Total                 |
| -----       |            |             |                       |
| 100.0%      | 623.115490 | 2.0         | vhone_                |
| 100.0%      | 622.866674 | --          | vhone_.LOOP.2.li.205  |
| -----       |            |             |                       |
| 3   37.5%   | 233.441869 | 50.0        | sweepz_               |
| -----       |            |             |                       |
| 4    23.6%  | 147.324792 | --          | sweepz_.LOOP.05.li.53 |
| 5           |            |             | sweepz_.LOOP.06.li.54 |
| 6           |            |             | ppmlr_                |
| -----       |            |             |                       |
| 7      9.5% | 58.970451  | 819,200.0   | remap_                |
| -----       |            |             |                       |
| 8      5.8% | 35.940023  | 4,915,200.0 | parabola_             |
| 8      2.9% | 18.356531  | 819,200.0   | remap_(exclusive)     |
| =====       |            |             |                       |
| 7      7.7% | 47.983811  | 819,200.0   | riemann_              |
| 7      2.9% | 17.979033  | 2,457,600.0 | parabola_             |
| 7      1.7% | 10.292367  | 819,200.0   | evolve_               |
| =====       |            |             |                       |
| 4    13.8%  | 86.117076  | 50.0        | sweepz_(exclusive)    |
| =====       |            |             |                       |

Parallized Loop

# If it Vectorizes, Check Memory Utilization

|     |        |                                                                    |   |      |      |      |       |         |
|-----|--------|--------------------------------------------------------------------|---|------|------|------|-------|---------|
| 44. | V----  | do n = nmin-1, nmax                                                | 4 | 0.1% | 3.4  | 5.6  | 62.0% | line.44 |
| 45. | V      | ar(n) = a(n) + para(n,1)*dffa(n) + para(n,2)*da(n+1) + para(n,3)*d | 4 | 2.5% | 88.5 | 27.5 | 23.8% | line.45 |
| 48. | V      | al(n+1) = ar(n)                                                    | 4 | 0.2% | 7.1  | 8.9  | 56.0% | line.48 |
| 49. | V----  | enddo                                                              | 4 | 0.0% | 0.1  | 1.9  | 94.9% | line.49 |
| 53. | fV---- | do n = nmin, nmax                                                  | 4 | 0.3% | 9.6  | 10.4 | 52.3% | line.53 |
| 54. | fV     | onemfl= 1.0 - flat(n)                                              | 4 | 0.3% | 10.1 | 10.9 | 51.9% | line.54 |
| 55. | fV     | ar(n) = flat(n) * a(n) + onemfl * ar(n)                            | 4 | 0.9% | 31.3 | 14.7 | 32.0% | line.55 |
| 56. | fV     | al(n) = flat(n) * a(n) + onemfl * al(n)                            | 4 | 0.2% | 7.3  | 11.7 | 61.6% | line.56 |
| 57. | fV---- | enddo                                                              | 4 | 0.0% | 0.2  | 1.8  | 90.6% | line.57 |
| 67. | f----  | do n = nmin, nmax                                                  | 4 | 0.4% | 13.6 | 10.4 | 43.5% | line.68 |
| 68. | f      | deltaa(n) = ar(n) - al(n)                                          | 4 | 0.8% | 27.2 | 13.8 | 33.9% | line.69 |
| 69. | f      | a6(n) = 6. * (a(n) - .5 * (al(n) + ar(n)))                         | 4 | 0.4% | 15.4 | 11.6 | 43.2% | line.70 |
| 70. | f      | scrch1(n) = (ar(n) - a(n)) * (a(n)-al(n))                          | 4 | 0.4% | 13.4 | 10.6 | 44.3% | line.71 |
| 71. | f      | scrch2(n) = deltaa(n) * deltaa(n)                                  | 4 | 0.4% | 14.0 | 12.0 | 46.2% | line.72 |
| 72. | f      | scrch3(n) = deltaa(n) * a6(n)                                      | 4 | 0.1% | 4.8  | 8.2  | 63.5% | line.75 |
| 73. | f----  | enddo                                                              | 4 | 0.3% | 10.2 | 9.8  | 49.1% | line.76 |
| 74. | Vr2--  | do n = nmin, nmax                                                  | 4 | 0.6% | 19.4 | 14.6 | 43.1% | line.77 |
| 75. | Vr2    | if(scrch1(n) <= 0.0) then                                          | 4 | 0.5% | 17.9 | 11.1 | 38.4% | line.78 |
| 77. | Vr2    | ar(n) = a(n)                                                       | 4 | 1.2% | 40.6 | 16.4 | 28.8% | line.80 |
| 78. | Vr2    | al(n) = a(n)                                                       | 4 | 1.8% | 63.9 | 24.1 | 27.5% | line.81 |
| 79. | Vr2    | endif                                                              | 4 | 0.0% | 0.2  | 2.8  | 92.7% | line.82 |
| 80. | Vr2    | if(scrch2(n) < +scrch3(n)) al(n) = 3. * a(n) - 2. * ar(n)          | 4 | 0.1% | 4.3  | 7.7  | 64.4% | line.84 |
| 81. | Vr2    | if(scrch2(n) < -scrch3(n)) ar(n) = 3. * a(n) - 2. * al(n)          | 4 | 0.5% | 16.0 | 12.0 | 43.2% | line.85 |
| 82. | Vr2--> | enddo                                                              | 4 | 0.6% | 21.3 | 13.7 | 39.4% | line.86 |
| 83. | Vr2--  | do n = nmin, nmax                                                  | 4 | 0.0% | 0.0  | 1.0  | 95.7% | line.87 |
| 84. | Vr2    | deltaa(n)= ar(n) - al(n)                                           |   |      |      |      |       |         |
| 85. | Vr2    | a6(n) = 6. * (a(n) - .5 * (al(n) + ar(n)))                         |   |      |      |      |       |         |
| 86. | Vr2    |                                                                    |   |      |      |      |       |         |
| 87. | Vr2--> | enddo                                                              |   |      |      |      |       |         |

PARABOLA







# If it Vectorizes, Check Memory Utilization

```
44. V----< do n = nmin-1, nmax
45. V      ar(n) = a(n) + para(n,1)*diffa(n) + para(n,2)*da(n+1) + para(n,3)*da(n)
48. V      al(n+1) = ar(n)
49. V----> enddo
53. fV----< do n = nmin, nmax
54. fV      onemfl= 1.0 - flat(n)
55. fV      ar(n) = flat(n) * a(n) + onemfl * ar(n)
56. fV      al(n) = flat(n) * a(n) + onemfl * al(n)
57. fV----> enddo
67. f----< do n = nmin, nmax
68. f      deltaa(n) = ar(n) - al(n)
69. f      a6(n) = 6. * (a(n) - .5 * (al(n) + ar(n)))
70. f      scrch1(n) = (ar(n) - a(n)) * (a(n)-al(n))
71. f      scrch2(n) = deltaa(n) * deltaa(n)
72. f      scrch3(n) = deltaa(n) * a6(n)
73. f----> enddo
74.
75. Vr2--< do n = nmin, nmax
76. Vr2      if(scrch1(n) <= 0.0) then
77. Vr2          ar(n) = a(n)
78. Vr2          al(n) = a(n)
79. Vr2      endif
80. Vr2      if(scrch2(n) < +scrch3(n)) al(n) = 3. * a(n) - 2. * ar(n)
81. Vr2      if(scrch2(n) < -scrch3(n)) ar(n) = 3. * a(n) - 2. * al(n)
82. Vr2--> enddo
83.
84. Vr2--< do n = nmin, nmax
85. Vr2      deltaa(n)= ar(n) - al(n)
86. Vr2      a6(n) = 6. * (a(n) - .5 * (al(n) + ar(n)))
87. Vr2--> enddo
```

Remove unnecessary arrays  
and fuse loops

```
52. Vr2--< do n = nmin, nmax
53. Vr2      onemfl= 1.0 - flat(n)
54. Vr2      ar(n) = flat(n) * a(n) + onemfl * ar(n)
55. Vr2      al(n) = flat(n) * a(n) + onemfl * al(n)
56. Vr2      deltaa(n) = ar(n) - al(n)
57. Vr2      a6(n) = 6. * (a(n) - .5 * (al(n) + ar(n)))
58. Vr2      scrch1s = (ar(n) - a(n)) * (a(n)-al(n))
59. Vr2      scrch2s = deltaa(n) * deltaa(n)
60. Vr2      scrch3s = deltaa(n) * a6(n)
61. Vr2      if(scrch1s <= 0.0) then
62. Vr2          ar(n) = a(n)
63. Vr2          al(n) = a(n)
64. Vr2      endif
65. Vr2      if(scrch2s < +scrch3s) al(n) = 3. * a(n) - 2. * ar(n)
66. Vr2      if(scrch2s < -scrch3s) ar(n) = 3. * a(n) - 2. * al(n)
67. Vr2      deltaa(n)= ar(n) - al(n)
68. Vr2      a6(n) = 6. * (a(n) - .5 * (al(n) + ar(n)))
69. Vr2--> enddo
```



# If it Doesn't Vectorize – Fix It

```
||||=====
|| 10.8% | 376.9 | -- | -- |riemann_
3|      |      |      |      | riemann.f90
||||-----
4||| 1.4% | 47.4 | 32.6 | 41.0% |line.77
4||| 3.9% | 135.8 | 28.2 | 17.3% |line.78
```

```
63. + 1----< do l = lmin, lmax
64. + 1 2--< do n = 1, 12
65.   1 2    pmold(l) = pmid(l)
66.   1 2    wlft(l) = 1.0 + gamfac1*(pmid(l) - plft(l)) * plfti(l)
67.   1 2    wrgh(l) = 1.0 + gamfac1*(pmid(l) - prgh(l)) * prghi(l)
68.   1 2    wlft(l) = clft(l) * sqrt(wlfti(l))
69.   1 2    wrgh(l) = crgh(l) * sqrt(wrghi(l))
70.   1 2    zlft(l) = 4.0 * vlft(l) * wlft(l) * wlfti(l)
71.   1 2    zrgh(l) = 4.0 * vrgh(l) * wrgh(l) * wrghi(l)
72.   1 2    zlft(l) = -zlft(l) * wlft(l)/(zlft(l) - gamfac2*(pmid(l) - plft(l)))
73.   1 2    zrgh(l) = zrgh(l) * wrgh(l)/(zrgh(l) - gamfac2*(pmid(l) - prgh(l)))
74.   1 2    umidl(l) = ulft(l) - (pmid(l) - plft(l)) / wlft(l)
75.   1 2    umidr(l) = urgh(l) + (pmid(l) - prgh(l)) / wrgh(l)
76.   1 2    pmid(l) = pmid(l) + (umidr(l) - umidl(l))*(zlft(l) * zrgh(l)) / (zrgh(l) - zlft(l))
77.   1 2    pmid(l) = max(smallp,pmid(l))
78.   1 2    if (abs(pmid(l)-pmold(l))/pmid(l) < tol ) exit
79.   1 2--> enddo
80. -1----> enddo
```

ftn-6254 ftn: VECTOR RIEMANN, File = riemann.f90, Line = 64

A loop starting at line 64 was not vectorized because a recurrence was found on "pmid" at line 77.



COMPUTE

STORE

ANALYZE

# If it Doesn't Vectorize – Fix It

```
63. + 1----< do l = lmin, lmax
64. + 1 2--< do n = 1, 12
65.   1 2    pmold(l) = pmid(l)
66.   1 2    wlft(l) = 1.0 + gamfac1*(pmid(l) - plft(l)) * plfti(l)
67.   1 2    wrgh(l) = 1.0 + gamfac1*(pmid(l) - prgh(l)) * prghi(l)
68.   1 2    wlft(l) = clft(l) * sqrt(wlft(l))
69.   1 2    wrgh(l) = crgh(l) * sqrt(wrgh(l))
70.   1 2    zlft(l) = 4.0 * vlft(l) * wlft(l) * wlft(l)
71.   1 2    zrgh(l) = 4.0 * vrgh(l) * wrgh(l) * wrgh(l)
72.   1 2    zlft(l) = -zlft(l) * wlft(l)/(zlft(l) - gamfac2*(pmid(l) - plft(l)))
73.   1 2    zrgh(l) = zrgh(l) * wrgh(l)/(zrgh(l) - gamfac2*(pmid(l) - prgh(l)))
74.   1 2    umidl(l) = ulft(l) - (pmid(l) - plft(l)) / wlft(l)
75.   1 2    umidr(l) = urgh(l) + (pmid(l) - prgh(l)) / wrgh(l)
76.   1 2    pmid(l) = pmid(l) + (umidr(l) - umidl(l))*(zlft(l) * zrgh(l)) /
                                     (zrgh(l) - zlft(l))
77.   1 2    pmid(l) = max(smallp,pmid(l))
78.   1 2    if (abs(pmid(l)-pmold(l))/pmid(l) < tol ) exit
79. 1 2--> enddo
80. 1----> enddo
```

```
62. A-----<> converged = .F.
63. + 1-----< do n = 1, 12
64.   1 Vr2--< do l = lmin, lmax
65.   1 Vr2    if(.not.converged(l))then
66.   1 Vr2    pmold(l) = pmid(l)
67.   1 Vr2    wlft(l) = 1.0 + gamfac1*(pmid(l) - plft(l)) * plfti(l)
68.   1 Vr2    wrgh(l) = 1.0 + gamfac1*(pmid(l) - prgh(l)) * prghi(l)
69.   1 Vr2    wlft(l) = clft(l) * sqrt(wlft(l))
70.   1 Vr2    wrgh(l) = crgh(l) * sqrt(wrgh(l))
71.   1 Vr2    zlft(l) = 4.0 * vlft(l) * wlft(l) * wlft(l)
72.   1 Vr2    zrgh(l) = 4.0 * vrgh(l) * wrgh(l) * wrgh(l)
73.   1 Vr2    zlft(l) = -zlft(l) * wlft(l)/(zlft(l) - gamfac2*(pmid(l) - plft(l)))
74.   1 Vr2    zrgh(l) = zrgh(l) * wrgh(l)/(zrgh(l) - gamfac2*(pmid(l) - prgh(l)))
75.   1 Vr2    umidl(l) = ulft(l) - (pmid(l) - plft(l)) / wlft(l)
76.   1 Vr2    umidr(l) = urgh(l) + (pmid(l) - prgh(l)) / wrgh(l)
77.   1 Vr2    pmid(l) = pmid(l) + (umidr(l) - umidl(l))*(zlft(l) * zrgh(l)) / &
                                     (zrgh(l) - zlft(l))
78.   1 Vr2    pmid(l) = max(smallp,pmid(l))
79.   1 Vr2
80.   1 Vr2    if (abs(pmid(l)-pmold(l))/pmid(l) < tol ) then
81.   1 Vr2    converged(l) = .T.
82.   1 Vr2    endif
83.   1 Vr2    endif
84.   1 Vr2--> enddo
85. + 1    if(all(converged(lmin:lmax)))exit
86. 1-----> enddo
```

# SWEEPZ

```
|| 10.3% | 1,679.0 | -- | -- | sweepz_  
3|      |      |      |      |      | levesque/CUG_2018/VH1_version1/sweepz.f90  
| | | |-----  
4| | | 3.0% | 489.4 | 21.6 | 4.3% | line.27  
4| | | 1.3% | 211.9 | 38.1 | 15.4% | line.64  
4| | | 1.0% | 165.0 | 43.0 | 20.8% | line.104  
4| | | 2.7% | 447.2 | 36.8 | 7.7% | line.121
```

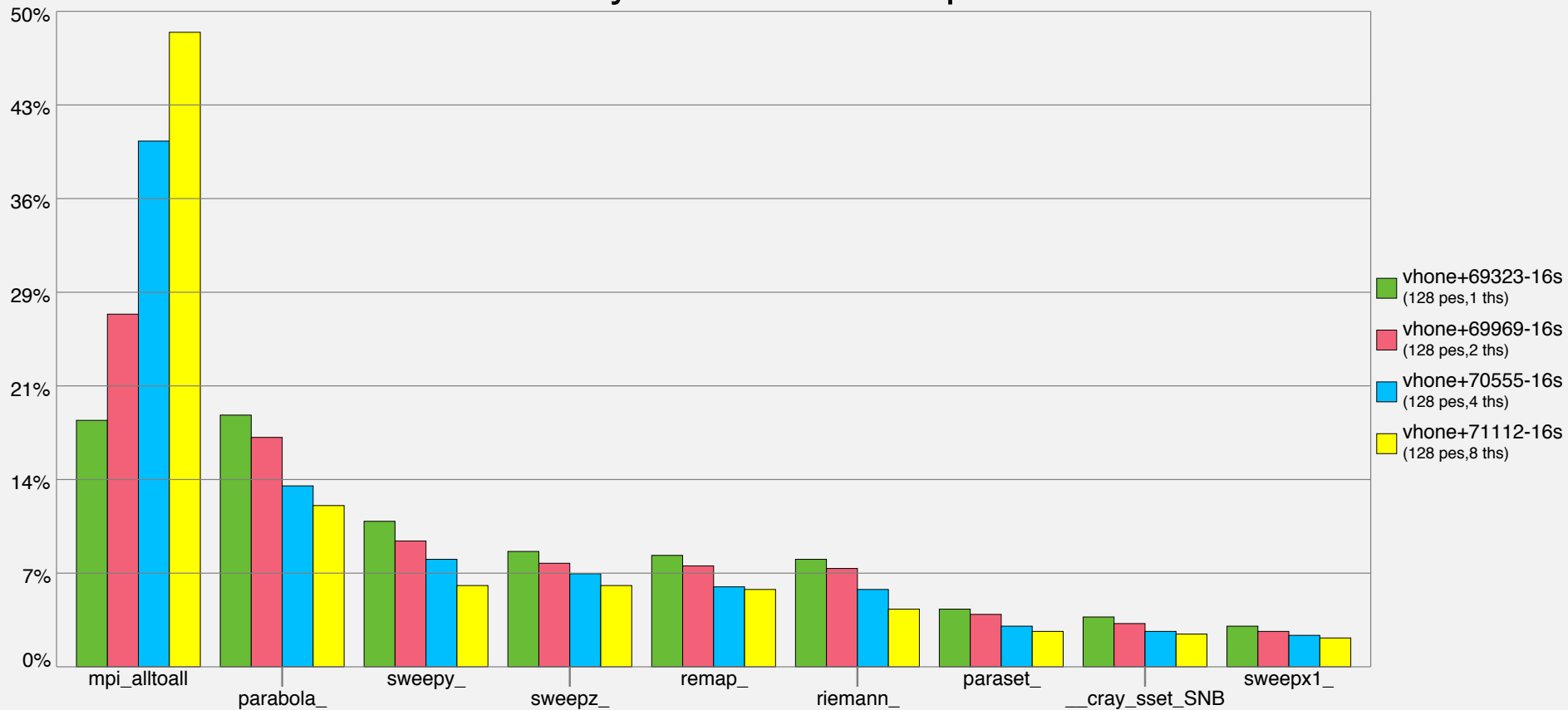
# SWEEPZ

```
22.  + i-----< do j = 1, js
23.  + i i-----< do m = 1, npey
24.  + i i i-----< do i = 1, isy
25.    i i i          n = i + isy*(m-1)
26.  + i i i 4-----< do k = 1, ks
27.    i i i 4 VR--<>    send3(1,j,k,n) = recv2(1,k,i,j,m)
28.    i i i 4          send3(2,j,k,n) = recv2(2,k,i,j,m)
29.    i i i 4          send3(3,j,k,n) = recv2(3,k,i,j,m)
30.    i i i 4          send3(4,j,k,n) = recv2(4,k,i,j,m)
31.    i i i 4          send3(5,j,k,n) = recv2(5,k,i,j,m)
32.    i i i 4          send3(6,j,k,n) = recv2(6,k,i,j,m)
33.    i i i 4----->    enddo
34.    i i i----->    enddo
35.    i i----->    enddo
36.    i----->    enddo
```

# SWEEPZ (continued)

```
21.                                     !-----
22.      M-----< !$OMP PARALLEL DO
23.  + M im-----< do j = 1, js
24.  + M im i-----< do m = 1, npey
25.  + M im i i-----< do i = 1, isy
26.      M im i i          n = i + isy*(m-1)
27.  + M im i i 5-----< do k = 1, ks
28.      M im i i 5 VR--<>      send3(1,j,k,n) = recv2(1,k,i,j,m)
29.      M im i i 5          send3(2,j,k,n) = recv2(2,k,i,j,m)
30.      M im i i 5          send3(3,j,k,n) = recv2(3,k,i,j,m)
31.      M im i i 5          send3(4,j,k,n) = recv2(4,k,i,j,m)
32.      M im i i 5          send3(5,j,k,n) = recv2(5,k,i,j,m)
33.      M im i i 5          send3(6,j,k,n) = recv2(6,k,i,j,m)
34.      M im i i 5----->      enddo
35.      M im i i----->      enddo
36.      M im i----->      enddo
37.      M im----->>      enddo
```

# Routines by Percent of Samples



# Profile for 1 Thread and 4 Threads

Table 1: Profile by Function 1 Thread

| Samp%  | Samp     | Imb.    | Imb.  | Group                       |
|--------|----------|---------|-------|-----------------------------|
|        |          | Samp    | Samp% | Function=[MAX10]<br>PE=HIDE |
| 100.0% | 38,034.0 | --      | --    | Total                       |
| -----  |          |         |       |                             |
| 73.5%  | 27,936.5 | --      | --    | USER                        |
| -----  |          |         |       |                             |
| 19.2%  | 7,320.6  | 202.4   | 2.7%  | parabola_                   |
| 11.1%  | 4,206.8  | 179.2   | 4.1%  | sweepy_                     |
| 8.8%   | 3,350.8  | 233.2   | 6.6%  | sweepz_                     |
| 8.5%   | 3,231.5  | 138.5   | 4.1%  | remap_                      |
| 8.2%   | 3,106.3  | 2,321.7 | 43.1% | riemann_                    |
| 4.4%   | 1,660.7  | 105.3   | 6.0%  | paraset_                    |
| 3.1%   | 1,190.9  | 72.1    | 5.8%  | sweepx1_                    |
| 3.0%   | 1,136.4  | 68.6    | 5.7%  | sweepx2_                    |
| =====  |          |         |       |                             |
| 20.5%  | 7,814.0  | --      | --    | MPI                         |
| -----  |          |         |       |                             |
| 18.8%  | 7,159.8  | 835.2   | 10.5% | mpi_alltoall                |
| =====  |          |         |       |                             |

Table 1: Profile by Function 4 threads

| Samp%  | Samp     | Imb.  | Imb.  | Group                                      |
|--------|----------|-------|-------|--------------------------------------------|
|        |          | Samp  | Samp% | Function=[MAX10]<br>PE=HIDE<br>Thread=HIDE |
| 100.0% | 15,265.8 | --    | --    | Total                                      |
| -----  |          |       |       |                                            |
| 54.1%  | 8,260.7  | --    | --    | USER                                       |
| -----  |          |       |       |                                            |
| 13.8%  | 2,101.9  | 84.1  | 3.9%  | parabola_                                  |
| 8.2%   | 1,252.8  | 62.2  | 4.8%  | sweepy_                                    |
| 7.1%   | 1,090.2  | 63.8  | 5.6%  | sweepz_                                    |
| 6.1%   | 926.8    | 62.2  | 6.3%  | remap_                                     |
| 5.9%   | 901.4    | 712.6 | 44.5% | riemann_                                   |
| 3.1%   | 480.2    | 71.8  | 13.1% | paraset_                                   |
| 2.4%   | 359.3    | 49.7  | 12.3% | sweepx1_                                   |
| 2.2%   | 329.7    | 46.3  | 12.4% | sweepx2_                                   |
| =====  |          |       |       |                                            |
| 41.4%  | 6,326.9  | --    | --    | MPI                                        |
| -----  |          |       |       |                                            |
| 40.1%  | 6,120.0  | 209.0 | 3.3%  | mpi_alltoall                               |
| =====  |          |       |       |                                            |



# Memory Analysis for Optimized VH1



Table 5: Profile by Group, Function, and Line

| Samp%  | Samp  | Imb. | Imb.  | MEM_LOAD_UOPS_RETIRED  | RESOURCE_STALLS       | Group                      |
|--------|-------|------|-------|------------------------|-----------------------|----------------------------|
|        |       | Samp | Samp% | :HIT_LFB:precise=2     | :ANY                  | Function=[MAX10]<br>Source |
|        |       |      |       |                        |                       | Line<br>PE=HIDE            |
| 100.0% | 506.4 | --   | --    | 52,444,505,648,539,880 | 810,810,111,305       | Total                      |
| -----  |       |      |       |                        |                       |                            |
| 67.0%  | 339.1 | --   | --    | 35,351,497,873,955,312 | 551,686,946,473       | USER                       |
| -----  |       |      |       |                        |                       |                            |
| 25.6%  | 129.5 | --   | --    | 13,561,376,423,707,960 | 207,864,527,154       | parabola_                  |
| 3      |       |      |       |                        |                       | parabola.f90               |
| -----  |       |      |       |                        |                       |                            |
| 4      | 14.0% | 71.1 | 77.9  | 52.7%                  | 7,540,450,746,779,697 | 113,994,086,387   line.26  |
| 4      | 1.0%  | 5.2  | 8.8   | 63.0%                  | 510,173,395,620,708   | 8,400,427,348   line.32    |
| 4      | 8.1%  | 41.0 | 41.0  | 50.4%                  | 4,241,915,862,200,189 | 65,974,673,046   line.46   |
| 4      | 1.3%  | 6.8  | 9.2   | 58.0%                  | 714,682,558,419,997   | 10,882,073,895   line.55   |
| =====  |       |      |       |                        |                       |                            |
|        | 12.1% | 61.2 | --    | --                     | 6,449,735,211,652,689 | 103,694,034,743   sweepy_  |
| 3      |       |      |       |                        |                       | sweepy.f90                 |
| -----  |       |      |       |                        |                       |                            |
| 4      | 3.2%  | 16.2 | 19.8  | 55.6%                  | 1,653,665,489,088,910 | 27,467,001,609   line.46   |
| 4      | 6.4%  | 32.2 | 34.8  | 52.4%                  | 3,465,660,652,265,039 | 54,562,573,915   line.47   |
| =====  |       |      |       |                        |                       |                            |
|        | 10.2% | 51.9 | --    | --                     | 5,479,965,955,430,281 | 81,379,551,948   sweepz_   |
| 3      |       |      |       |                        |                       | sweepz.f90                 |
| -----  |       |      |       |                        |                       |                            |
| 4      | 2.4%  | 12.3 | 19.7  | 62.0%                  | 1,356,797,349,204,156 | 21,098,054,630   line.28   |
| 4      | 1.8%  | 8.9  | 13.1  | 60.0%                  | 945,580,000,330,081   | 13,804,851,073   line.65   |
| 4      | 3.7%  | 18.8 | 28.2  | 60.4%                  | 1,961,528,744,947,444 | 29,502,970,062   line.66   |

COMPUTE | STORE | ANALYZE

# Code Responsible for Memory Bandwidth

```
24.      !-----  
25.      Vr4---<    do n = nmin-2, nmax+1  
26.      Vr4          diffa(n) = a(n+1) - a(n)  
27.      Vr4--->    enddo  
28.  
29.      !                                                    Equation 1.7 of C&W  
30.      !          da(j) = D1 * (a(j+1) - a(j)) + D2 * (a(j) - a(j-1))  
31.      fVr4---<    do n = nmin-1, nmax+1  
32.      fVr4          da(n) = para(n,4) * diffa(n) + para(n,5) * diffa(n-1)  
33.      fVr4          da(n) = sign( min(abs(da(n)), 2.0*abs(diffa(n-1))), 2.0*abs(diffa(n))), da(n) )  
34.      fVr4--->    enddo  
35.  
36.      !          zero out da(n) if a(n) is a local max/min  
37.      f-----<    do n = nmin-1, nmax+1  
38.      f          if(diffa(n-1)*diffa(n) < 0.0) da(n) = 0.0  
39.      f----->    enddo  
40.  
41.      !                                                    Equation 1.6 of C&W  
42.      !          a(j+.5) = a(j) + C1 * (a(j+1)-a(j)) + C2 * dma(j+1) + C3 * dma(j)  
43.      ! MONOT: Limit ar(n) to the range defined by a(n) and a(n+1)  
44.  
45.      Vr2---<    do n = nmin-1, nmax  
46.      Vr2          ar(n) = a(n) + para(n,1)*diffa(n) + para(n,2)*da(n+1) + para(n,3)*da(n)  
47.      Vr2      !      ar(n) = max(ar(n),min(a(n),a(n+1)))  
48.      Vr2      !      ar(n) = min(ar(n),max(a(n),a(n+1)))  
49.      Vr2          al(n+1) = ar(n)  
50.      Vr2--->    enddo
```

Difficult to merge these loops – compiler  
did merge two

COMPUTE

STORE

ANALYZE

# Summary



- **The Whack-a-mole approach was shown to be an effective recipe for using the tools to obtain results**
- **Cray compiler and performance tools gives customers the capability they need to identify performance issues at scale in important production codes**
- **Simple interfaces coupled with a wealth of capability offer the most flexibility for users who need to scale applications to larger job and problem sizes**

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# Q&A

A scenic view of a historic city skyline, likely Stockholm, Sweden, featuring colorful buildings and a prominent church spire, reflected in the water.

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