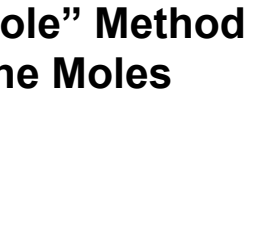
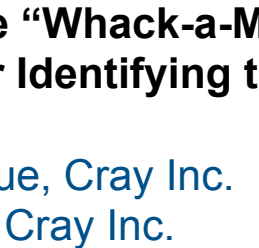
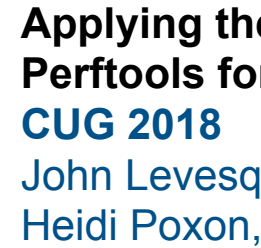
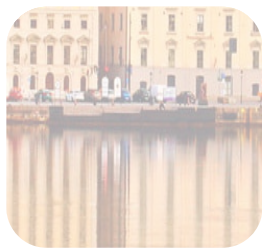


**CRAY**



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

**CUG 2018**

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

# 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)**

# 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**

The background of the central text is a photograph of a forest. The trees are tall and thin, with some appearing to be dead or charred, set against a blue sky with white clouds. The text is overlaid on this image.

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

Will Rogers

# Cray Performance Tools

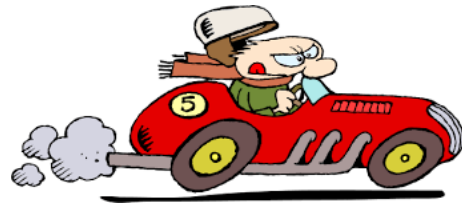
- **Reduce the time investment associated with porting and tuning applications on Cray systems**
- **Analyze whole-program behavior across many nodes to identify critical performance bottlenecks within a program**
- **Improve your profiling experience by using simple (lite mode) and/or advanced interfaces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

# Interfaces Available

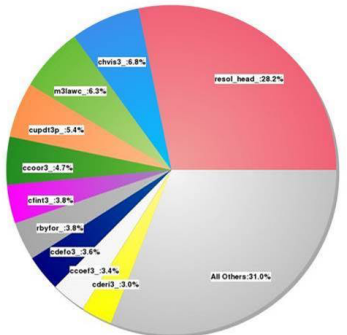
- **Simple interface (perftools-lite modes) for convenience**
- **Advanced interface (perftools) for in-depth performance investigation and tuning assistance as well as data collection control**
- **Both offer:**
  - Whole program analysis across many nodes
  - Indication of causes of problems
  - Ability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

**New!**

# pat\_run



**Profile pre-existing, dynamically linked programs**



Wallclock time: 720.229797s

**Collect different performance data for same binary**

**Get basic performance information on ISV codes**



# What is it?

*Utility that allows you to profile un-instrumented, dynamically linked binaries with CrayPat!*

- **Delivers Cray performance tools profiling information for codes that cannot be rebuilt**
  - **ISV codes** (where pre-built binaries or object files are supplied instead of source)
  - **Codes with long compile times**
- **Extends perftools ease-of-use and supports an even greater range of HPC applications**
  - OpenFoam was profiled successfully with pat\_run!

# pat\_run Advantages

- **Reduced steps to get application performance data**
- **No need to re-compile to obtain basic performance data**
- **Different performance experiments can be collected with the same binary**
- **No perftools modules required during compile or link**
- **Performance analysis on executable files stripped of their global symbol tables**

# Basic Usage

- Use `perftools-base/7.0.1` or later
- `aprun/srun -n 16 pat_run ./my_program`
  - Perform other experiments like
    - `pat_run -g mpi ./my_program`
- `pat_report exp_data_directory > my_report`
  - Use all of your favorite `pat_report` options, such as
    - `pat_report -P -O calltree`
    - `pat_report -s pe=ALL`

# Helpful perftools Experiments

- **Identify slowest areas and notable bottlenecks of a program**
  - Use **perftools-lite**
  - Good for examining performance characteristics of a program and for scaling analysis
- **Focus on loop optimization, including adding OpenMP with Reveal**
  - Use **perftools-lite-loops**
  - Use **perftools-lite-hbm** for memory bandwidth sensitivity study
- **Focus on MPI communication**
  - Use `perftools-lite` first to determine if MPI time is dominant or if there is a load imbalance between ranks
  - Use **perftools** (`pat_build -g mpi`) to collect more detailed MPI-specific information
  - Good for scaling analysis at targeted final job size



# Used in this Tutorial

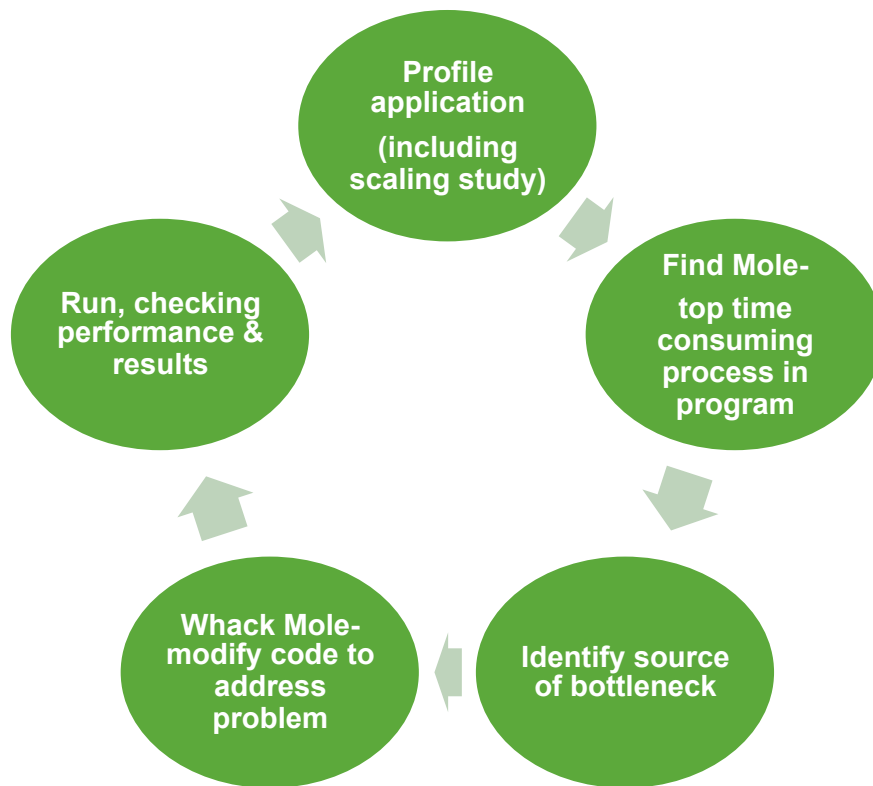
- **Several perftools-lite modes**
  - Simply load the desired module, compile, and execute program
- **Additional reports (`pat_report -O calltree`, etc.)**
- **perftools advanced interface**
  - Load `perftools` module and build program
  - Instrument program with `pat_build -u -g mpi`
  - Execute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

# 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)



COMPUTE

STORE

ANALYZE

# 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

# UMT Call Tree on 8 Nodes



Table 1. Call Tree View

Level	Inclusive Percent of Time	Exclusive Percent of Time	Time (s)	Leaf child routine-Exclusive Percent of Time
0	100.0%		3,971.6	Total
1	99.8%		3,961.9	main
2				main
3				main
4				main
5				main
6	66.9%		2,655.4	rswpmd_
7	66.8%		2,654.7	snflwxyz_
8		22.0%	872.3	exchange_
9		13.5%	535.7	MPI_WAIT
9		8.5%	336.5	exchange_(exclusive)
8		15.6%	617.7	snswp3d_
8		9.7%	383.4	initexchange
9				MPI_BARRIER
8		6.5%	260.0	snmoments_
8		5.8%	230.6	__cray_dcopy_HSW
8		4.0%	160.7	testfluxconv_
9				mpi_mpiallreduces_r_\$mpif90_m
10				MPI_ALLREDUCE
8		3.2%	128.7	setincidentflux_
6		21.6%	859.3	exchange_
7		15.6%	620.0	MPI_WAIT
7		6.0%	239.3	exchange_(exclusive)
5		5.0%	198.1	rtstrtsn_
6			106.9	rtstrtsn_(exclusive)
7			90.1	__cray_dcopy_HSW
8			115.2	advancert_
6		1.5%	60.0	advancert_(exclusive)
6		1.4%	55.2	snmoments_
2		1.0%	40.9	initialize

Nesting Level

Called From snflwxyz\_

Inclusive Percent of Time

Leaf child routine-Exclusive Percent of Time



# 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)

COMPUTE

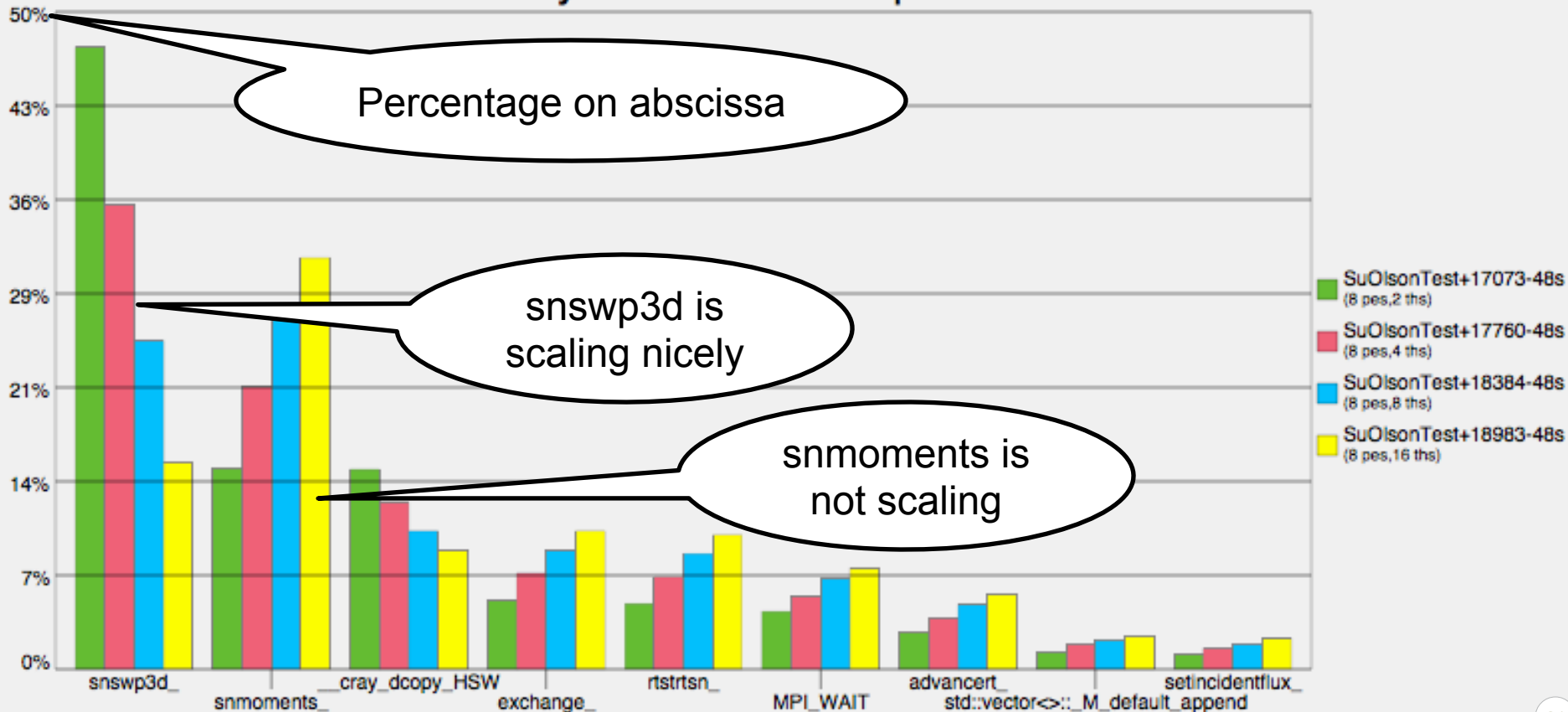
STORE

512 MPI tasks (1-4 OpenMP threads)

# UMT Scaling with MPI Tasks and OpenMP Threads



## Routines by Percent of Samples



Percentage on abscissa

snswp3d is scaling nicely

snmoments is not scaling

# 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.    1 2 M m          Angle = QuadSet% AngleOrder (mm,binSend)
109.    1 2 M m          thnum = 1
110.    1 2 M m          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 M m
114.  + 1 2 M m          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. 1
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





# Obtaining a Listing

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



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

	Loop Hit	Loop Trips Avg	Loop Trips Min	Loop Trips Max	Function=/.LOOP[.] PE=HIDE	
98.9%	52.728532	0.000069	1	7.0	7	main.LOOP.1.li.159
92.4%	52.728532	0.000154	7	4.7	3	rtmainsn_.LOOP.1.li.159
92.2%	52.728532	0.000114	33	1.0	1	rtmainsn_.LOOP.1.li.159
92.1%	52.647694	0.000214	33	1.0	1	rtmainsn_.LOOP.3.li.167
71.6%	40.965850	0.000417	33	1.6	1	snflwxyz_.LOOP.1.li.87
59.3%	33.937160	0.001694	54	6.9	4	snflwxyz_.LOOP.2.li.95
44.0%	25.175652	0.043310	90	2.8	1	snflwxyz_.LOOP.3.li.106
41.2%	23.541605	0.052865	28	8.4	1	snswp3d_.LOOP.01.li.78
28.2%	16.146745	3.884386	8	2.0	1	snswp3d_.LOOP.04.li.99
19.1%	10.931600	0.000059	8	1.4	1	exchange_.LOOP.06.li.120
19.1%	10.931541	10.931541	6	1.8	1	exchange_.LOOP.07.li.121
14.0%	7.993231	1.052804	7	1.4	1	snswp3d_.LOOP.08.li.132
11.9%	6.800924	6.800924	10	0.7	1	snswp3d_.LOOP.09.li.134
8.2%	4.692389	0.135064	8	5.9	1	snswp3d_.LOOP.05.li.110
8.0%	4.557325	4.557325	7,499,520	400.0	400	snswp3d_.LOOP.01.li.78
6.9%	3.944975	0.000352	405	5.0	3	exchange_.LOOP.08.li.132
6.9%	3.944623	1.409580	2,025	1.6	1	exchange_.LOOP.09.li.134
5.8%	3.312134	3.312134	7,499,520	3.0	3	snswp3d_.LOOP.05.li.110
5.0%	2.864861	0.003020	40	720.0	720	snmoments_.LOOP.1.li.58
5.0%	2.861841	0.051047	28,800	224.0	224	snmoments_.LOOP.2.li.64
4.9%	2.810795	2.810795	6,451,200	400.0	400	snmoments_.LOOP.3.li.65
4.7%	2.700843	0.000089	405	1.6	1	exchange_.LOOP.01.li.71

Ordered by loops that take most of the time

This is the loop with OpenMP



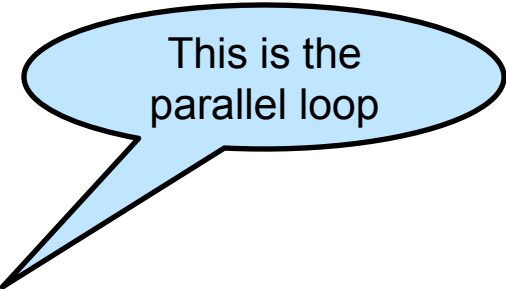
snmoments has nice loops lengths

# Profile Loops with Call Tree (1 of 2)

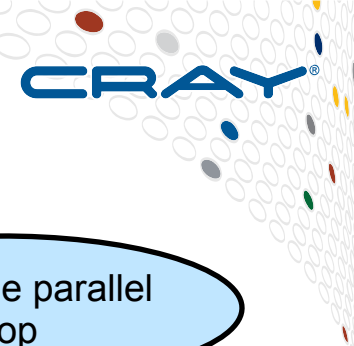
Table 1: Function Calltree View

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   rtmainstn_
-----			
7	92.5%	52.838008	--   rtmainstn_.LOOP.1.li.149
8	92.3%	52.719389	--   rtmainstn_.LOOP.2.li.159
9	92.1%	52.638677	--   rtmainstn_.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



# Profile Loops with Call Tree (2 of 2)



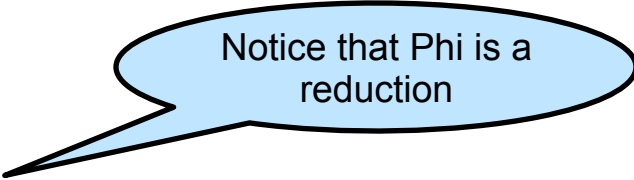
14		44.0%	25.123658	--	snflwxyz_.LOOP.3.li.106
15		43.4%	24.805902	33,480.0	snswp3d_
14		15.3%	8.759766	372.0	exchange_
=====					
13		8.0%	4.592279	54.0	initexchange_
13		2.9%	1.654016	54.0	testfluxconv_
13		1.4%	0.781868	54.0	setincidentflux_
=====					
12		4.1%	2.363264	33.0	snmoments_
=====					
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
```



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 Is 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 on 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...



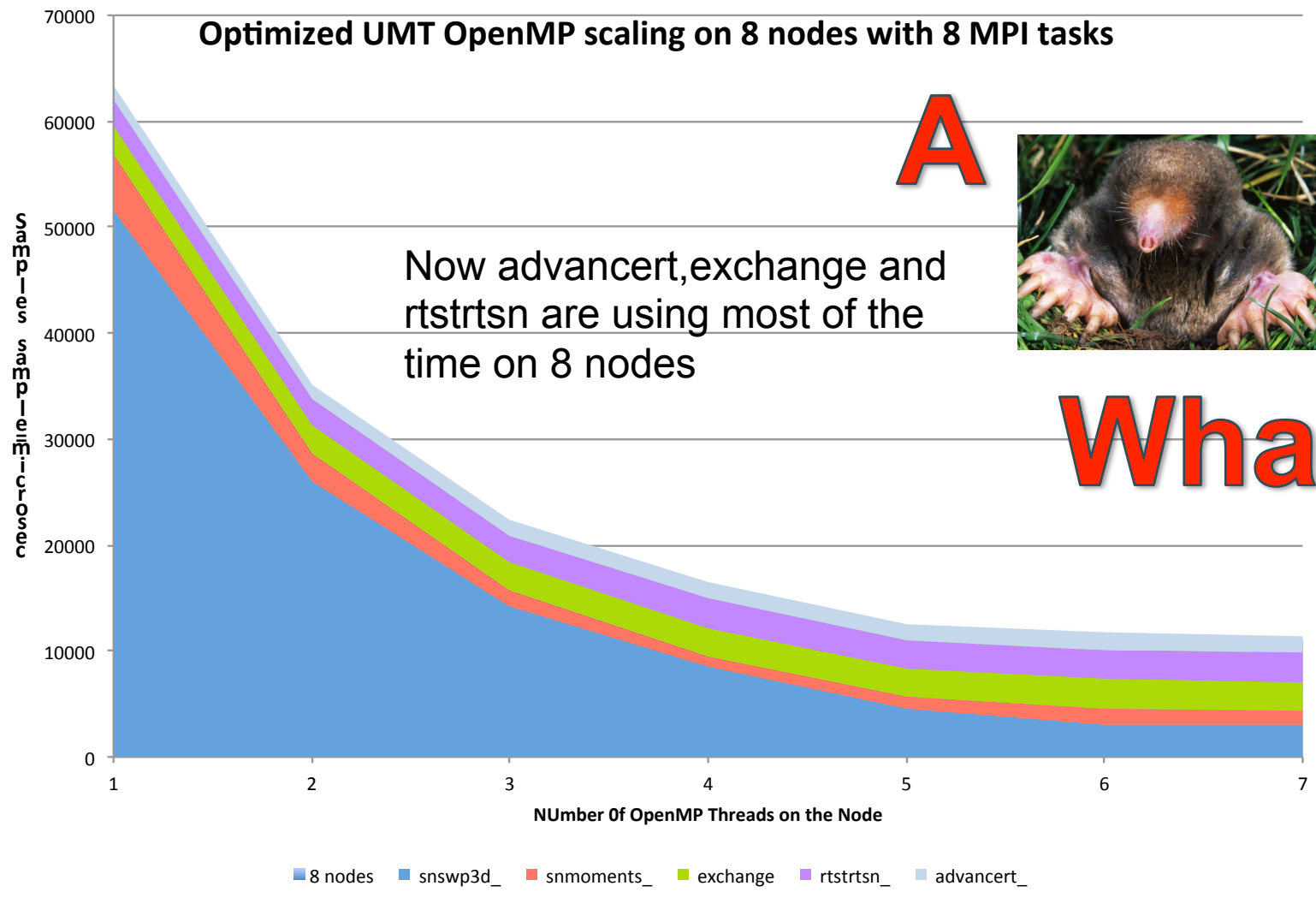
# Optimized UMT OpenMP scaling on 8 nodes with 8 MPI tasks

# A



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

# Whacked



# Major Loop in RTSTRTSN

<pre> 51.  + F-----&lt; 52.   F I 53.   F 54.   F 55.  + F 2-----&lt; 56.   F 2 C-----&lt; 57.   F 2 C VCr2----&lt;&gt; 58.   F 2 C-----&gt; 59.   F 2-----&gt; 60.   F-----&gt; </pre>	<pre> ZoneLoop: do zone=1,nzones           Z =&gt; 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 </pre>
---	---

# 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                vmessage(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 = vmessage(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



# 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

# 8 Node Configuration

Original      Optimized



Table 1: Profile by Function

Samp%	Samp	Imb. Samp	Imb. Samp%	Group
				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. Samp	Imb. Samp%	Group
				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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# 32 Node Configuration

Original    Optimized



Table 1: Profile by Function

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

Table 1: Profile by Function

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



# 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]
						Source
						Line
						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



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# 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
```

# 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



```
109.      F 2
110.      F 2 r6-----<
111.      F 2 r6
112.      F 2 r6
113.      F 2 r6
114.      F 2 r6
115.      F 2 r6
116.      F 2 r6
117.      F 2 r6
118.      F 2 r6
119.      F 2 r6
120.      F 2 r6
121.      F 2 r6
122.      F 2 r6 Vr2-----<
123.      F 2 r6 Vr2
124.      F 2 r6 Vr2
125.      F 2 r6 Vr2
126.      F 2 r6 Vr2
127.      F 2 r6 Vr2
128.      F 2 r6 Vr2
129.      F 2 r6 Vr2
130.      F 2 r6 Vr2----->
131.      F 2 r6
132.      F 2 r6----->
```

```
do icface=1,ncfaces

afpm(icface) = omega(1)*Z%A_fp
              omega(2)*Z%A_fp
              omega(3)*Z%A_fp

icfp      = Z%Connect(1,icface,c)
ib        = Z%Connect(2,icface,c)

if ( afpm(icface) >= zero ) then
  sumArea = sumArea + afpm(icface)
else
do ig = 1, Groups
  if (icfp == 0) then
    psifp(ig,icface) =
  else
    psifp(ig,icface) =
  endif
  src(ig,c) = src(ig,c)
enddo
endif
enddo
```

# Whacked

This simple change improved  
snswp3d by 50%

COMPUTE

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# Tips When Dealing with Big Applications

**Getting a Preview**



**Speeding up Report Generation**

**Controlling Amount of Data**



# Tips: Split .ap2 and Text Report Creation

- **Suppress serial report generation to speed up pat\_report processing time on compute nodes**
  - pat\_report automatically executed in perftools-lite mode
- **In execution environment, set**
  - PAT\_RT\_REPORT\_CMD='pat\_report,-Q0'
  - Good for talking to pat\_report when using perftools-lite
- **Works in lite and classic modes**



# Tips: Generate Report from Data Subset

- `pat_report -Q1 ...` Report from the first .ap2 file
- `pat_report -Q2 ...` Report from the first and last .ap2 file
- `pat_report -Q3 ...` Report from the first, middle, and last .ap2 file
- `-QN`: Select N .ap2 files, evenly distributed in the list of all .ap2 files

# Tips: Controlling Instrumentation and Data

- **Record Subset of PEs during execution**
  - Example: `export PAT_RT_EXPFILER_PES=0,4,5,10`
- **Don't instrument select binaries when using perftools-lite**
  - Good for applications that generate test or intermediate binaries with CMake and GNU Autotools
  - Use **CRAYPAT\_LITE\_WHITELIST** for binaries you DO want instrumented

# 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

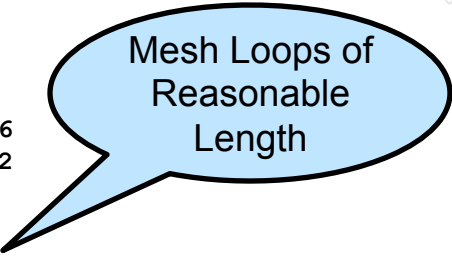
Time%	Time	Calls	Calltree
			PE=HIDE
100.0%	242.649260	--	Total
-----			
100.0%	242.649223	2.0	les3d_
99.2%	240.654228	--	les3d_.LOOP.3.li.216
-----			
97.9%	237.444979	--	les3d_.LOOP.4.li.272
-----			
29.1%	70.519335	4,000.0	fluxk_
-----			
17.7%	42.941276	--	fluxk_.LOOP.1.li.28
			fluxk_.LOOP.2.li.29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

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
<b>15.0%</b>	<b>36.464645</b>	<b>9,216,000.0   visci_</b>
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 Incl Time%	Loop Incl Time	Loop Hit	Loop Trips Avg	Loop Trips Min	Loop Trips Max	Function=/.LOOP[.] 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`
  - Reveal `<program library> <perftools statistics directory>`
    - Select one of the three high level loops in `fluxk`, `flukj`, `fluxi`

# 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 * IADD)
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)

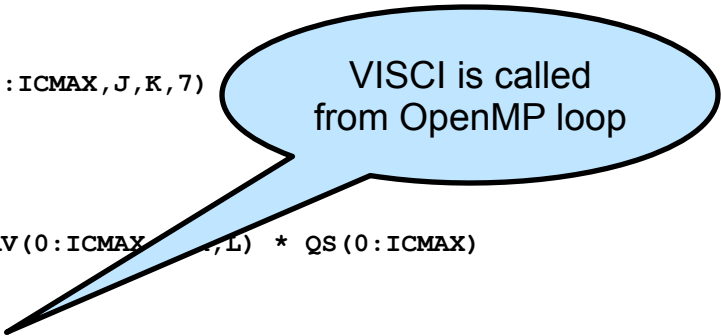
```
44.   M m 3 f-----<>
45.   M m 3 f-----<>
46.   M m 3                                     >
47.   M m 3 f-----<>
48.   M m 3                                     >
49.   M m 3 fVr2-----<>
50.   M m 3                                     >
51.   M m 3 f-----<>
52.   M m 3                                     >
53.   M m 3
54.   M m 3
55.   M m 3
56.   M m 3
57.   M m 3
58.   M m 3
59.   M m 3 D-----<
60.   M m 3 D
61.   M m 3 D----->
62.   M m 3
63.   M m 3
64. + M m 3
65.   M m 3
```

```
FSI(0:ICMAX,1) = QAV(0:ICMAX,J,K,1) * QS(0:ICMAX)
FSI(0:ICMAX,2) = QAV(0:ICMAX,J,K,2) * QS(0:ICMAX) +
                  PAV(0:ICMAX,J,K) * SIX(0:ICMAX,J,K)
FSI(0:ICMAX,3) = QAV(0:ICMAX,J,K,3) * QS(0:ICMAX) +
                  PAV(0:ICMAX,J,K) * SIY(0:ICMAX,J,K)
FSI(0:ICMAX,4) = QAV(0:ICMAX,J,K,4) * QS(0:ICMAX) +
                  PAV(0:ICMAX,J,K) * SIZ(0:ICMAX,J,K)
FSI(0:ICMAX,5) = (QAV(0:ICMAX,J,K,5) + PAV(0:ICMAX,J,K)) *
                  QS(0:ICMAX)

IF ( ISGSK .EQ. 1 ) THEN
  FSI(0:ICMAX,7) = QAV(0:ICMAX,J,K,7)
ENDIF

IF ( ICHEM .GT. 0 ) THEN
  DO L = 8, 7 + NSPECI
    FSI(0:ICMAX,L) = QAV(0:ICMAX,J,K,L) * QS(0:ICMAX)
  ENDDO
ENDIF

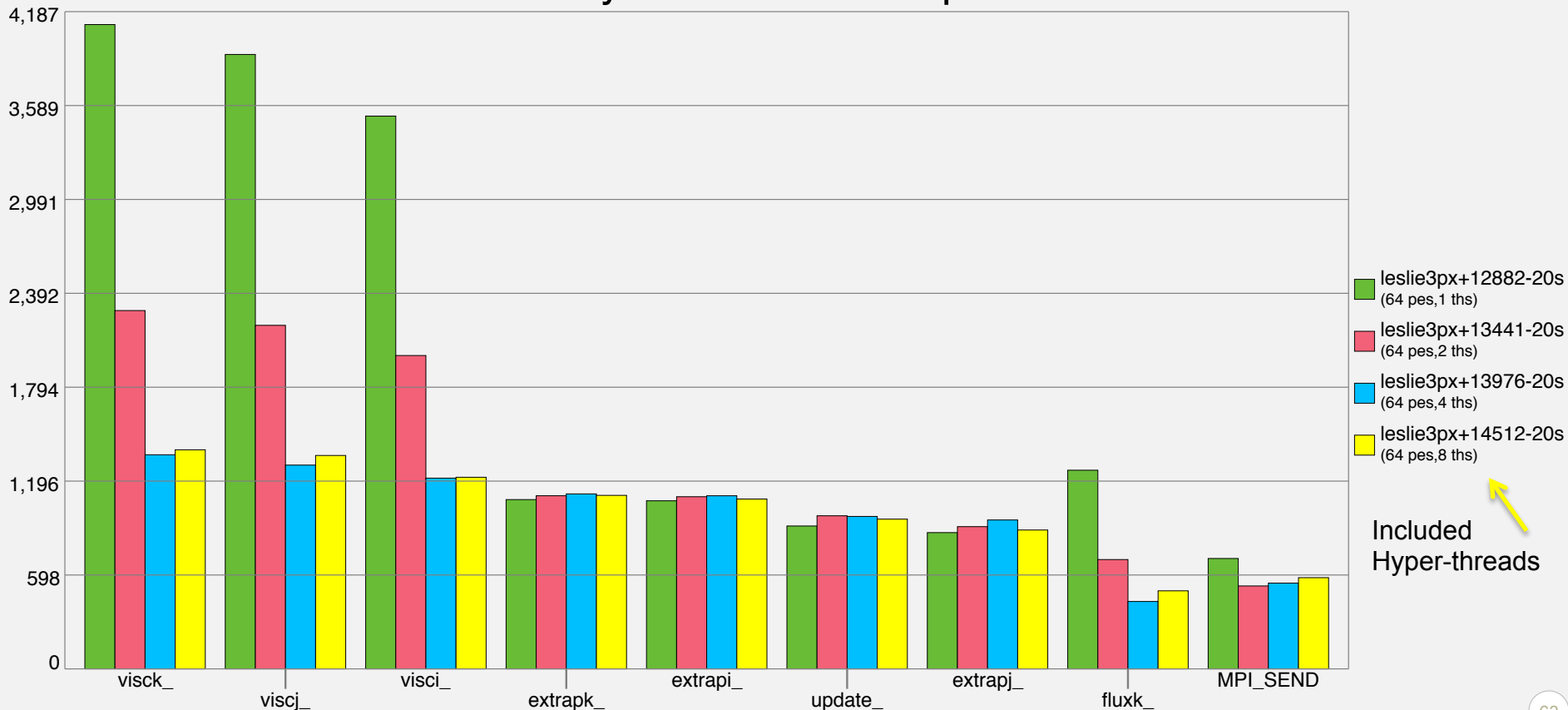
IF ( VISCOUS ) CALL VISCI ( 0, ICMAX, J, K, FSI )
```



VISCI is called  
from OpenMP loop

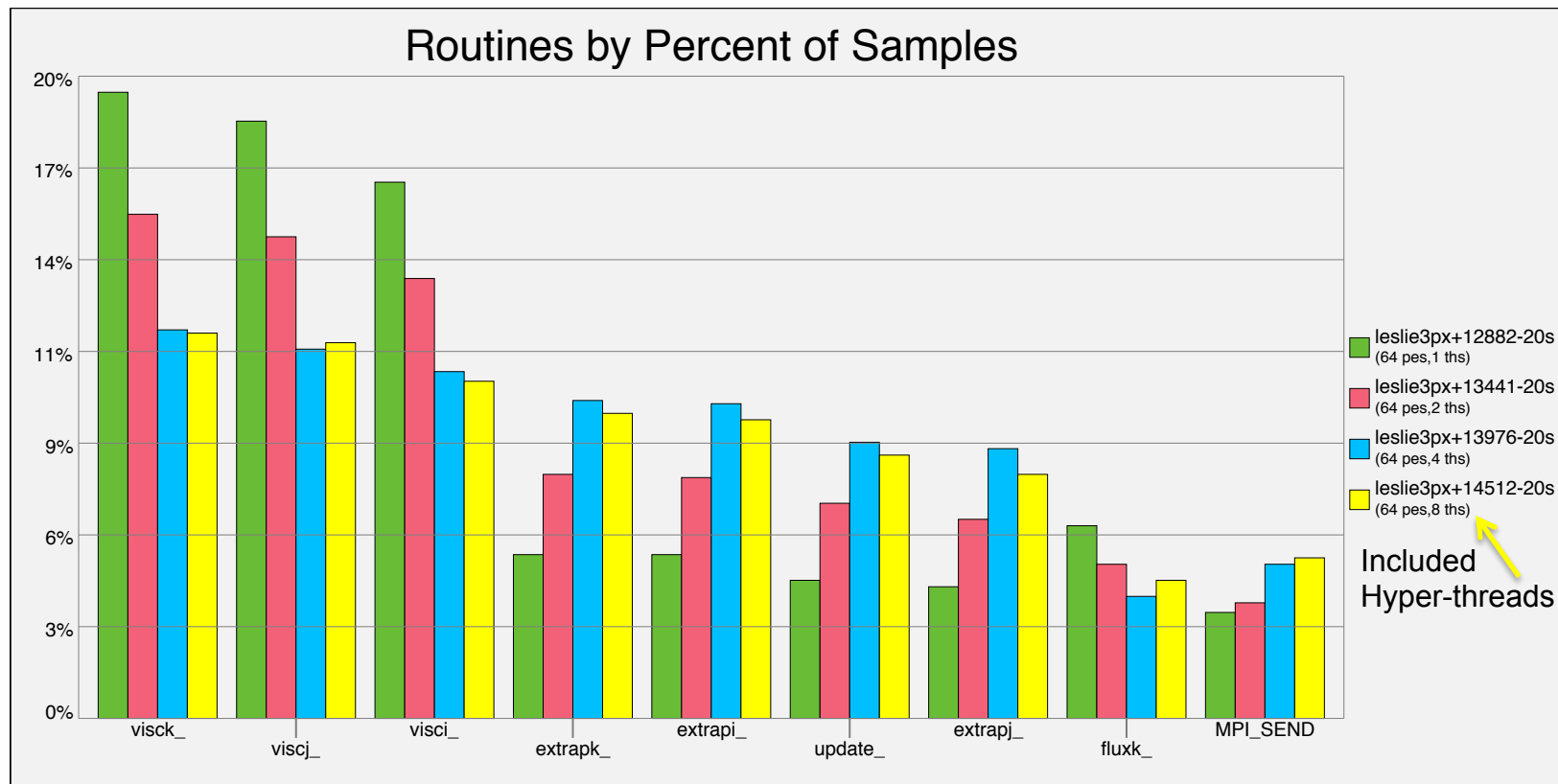
# 64 MPI Tasks on 8 Nodes

## Routines by Number of Samples



Included  
Hyper-threads

# 64 MPI Tasks on 8 Nodes



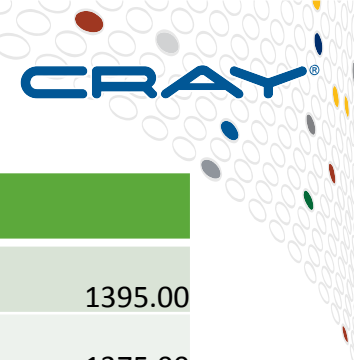
COMPUTE

STORE

ANALYZE



# Subroutine Timings After Parallelization of FLUXs



	1 Thread	2 Threads	4 Threads	8 Threads
visck_	4083.90	2270.40	1348.00	1395.00
viscj_	3859.10	2174.00	1292.40	1375.00
visci_	3805.60	2137.90	1281.70	1234.00
fluxk_	1273.00	696.00	429.90	492.00
extrapk_	1076.70	1099.90	1108.40	1098.00
fluxi_	1075.20	581.10	335.50	233.00
extrapi_	1074.00	1099.80	1091.10	1090.00
fluxj_	1050.80	562.70	318.00	227.00
update_	902.80	966.50	971.30	957.00
extrapj_	862.00	896.60	932.00	882.00

COMPUTE

STORE

ANALYZE

# 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)



# 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 = 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
<

```

```

--
>
>
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>

```



```

      K, 3 ) * DUDXI
      K, 3 ) * DVDXI
      K, 3 ) * DWDXI
      K, 3 ) * DTDXI
      DUDY ( I ) = T21 ( I, J, K, 3 ) * DUDXI
      DVY ( I ) = T21 ( I, J, K, 3 ) * DVDXI
      DWY ( I ) = T21 ( I, J, K, 3 ) * DWDXI
      DTI ( 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,N)
16.   1 2 iVbr4          ELSE
17. + 1 2 iVbr4 ib--<>          Q(I,J,K,1:5,M) = Q(I,J,K,1:5,N) +
18.   1 2 iVbr4          >          Q(I,J,K,1:5,N) + DQ(I,J,K,1:5)
19.   1 2 iVbr4          ENDIF
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----->          COMPUTE ENDDO
33.   1----->          STORE | ANALYZE

```





# 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))
```

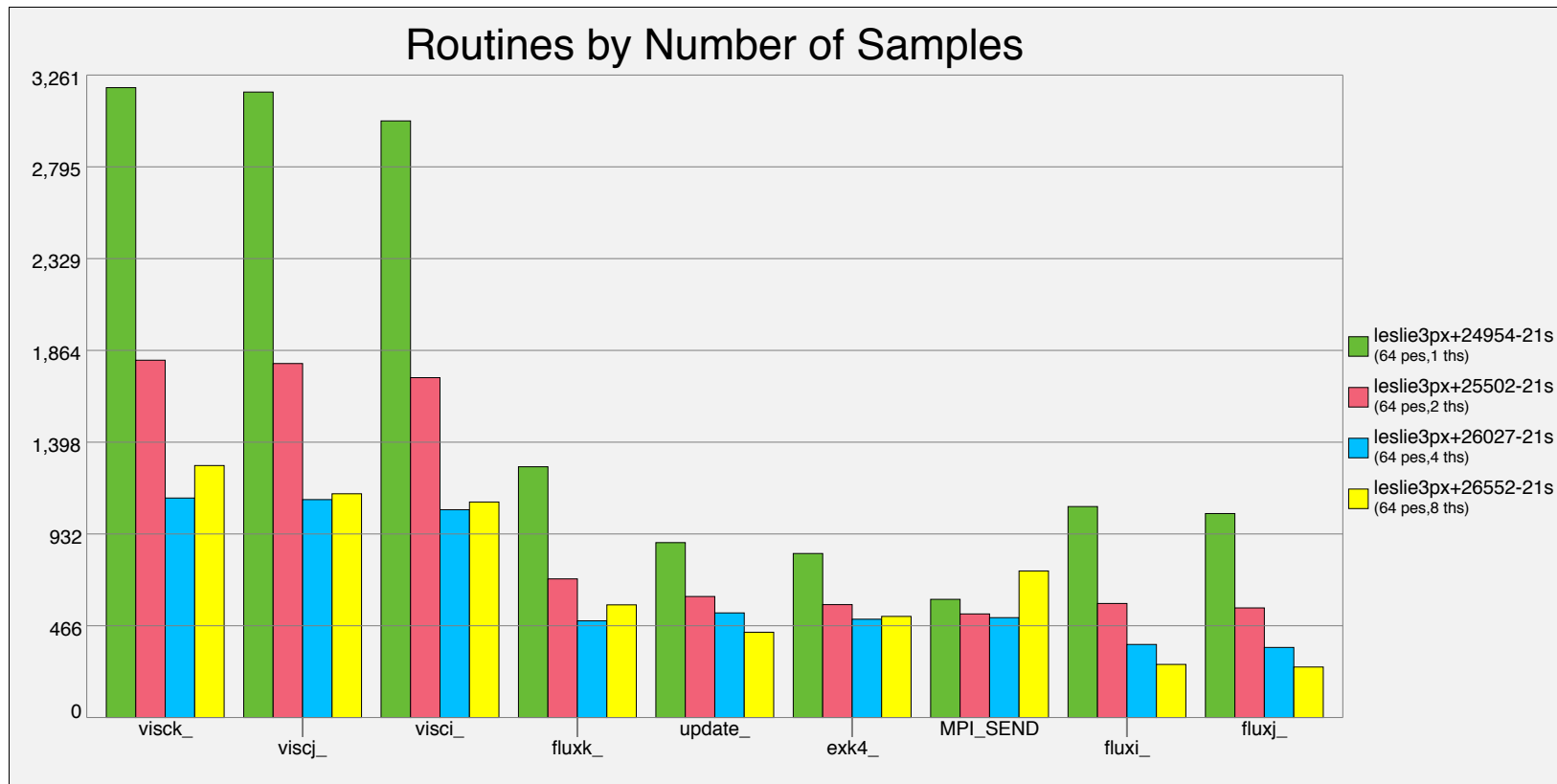
# Whacked

COMPUTE

STORE

ANALYZE

# Optimization Results for 64 MPI Tasks on 8 Nodes

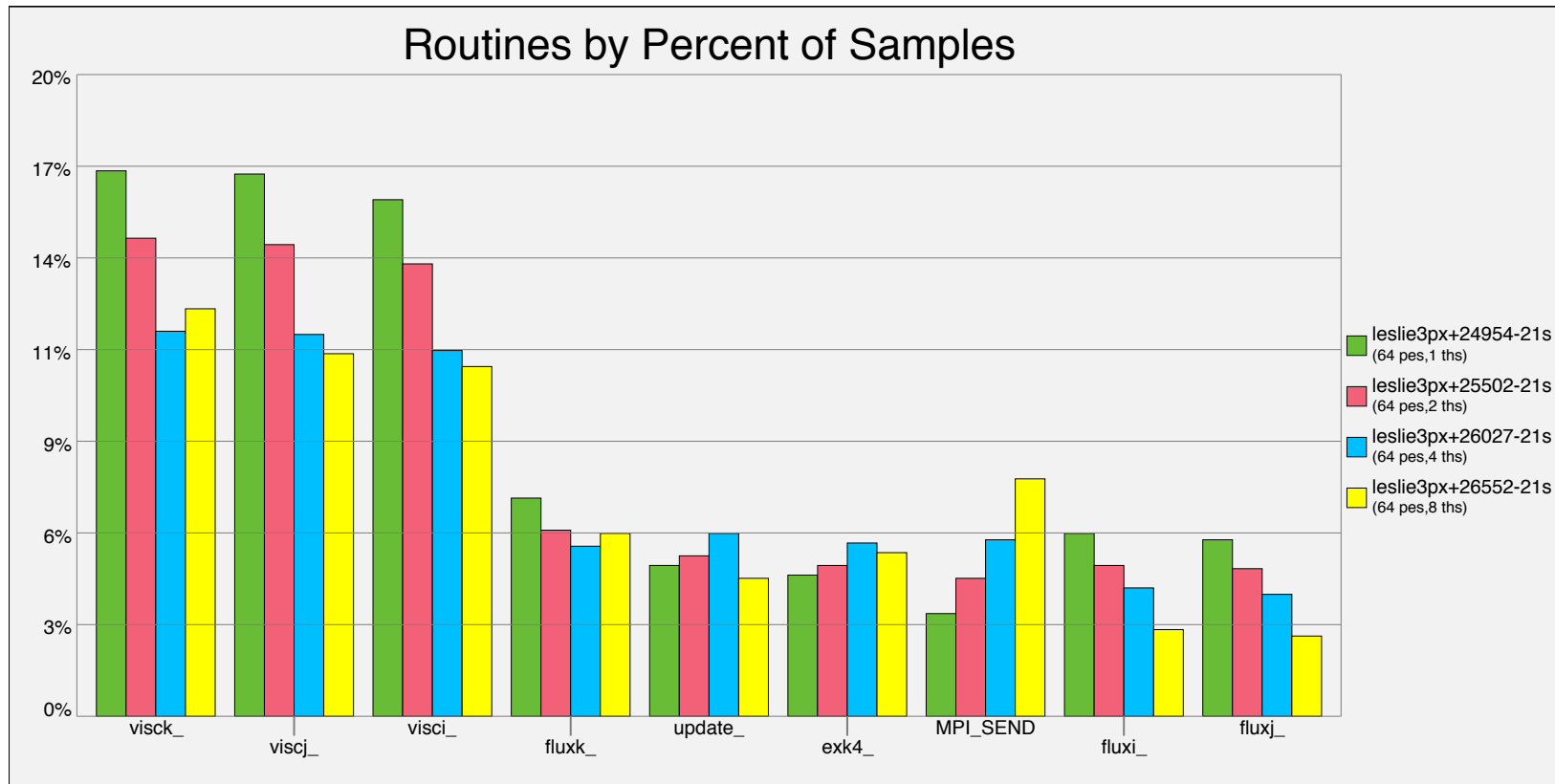


COMPUTE

STORE

ANALYZE

# Optimization Results for 64 MPI Tasks on 8 Nodes



COMPUTE

STORE

ANALYZE

# Final Sampling Profile



Table 1: Profile by Function

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

Table 1: Profile by Function

Samp%	Samp	Imb.	Imb.	Group
		Samp	Samp%	Function
				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_

## ORIGINAL

Table 1: Profile by Function

Samp%	Samp	Imb.	Imb.	Group
		Samp	Samp%	Function
				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

# 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. Samp	Imb. Samp%	MEM_LOAD_UOPS_RETIRED :HIT_LFB:precise=2	RESOURCE_STALLS :ANY	Group Function=[MAX10] Source Line 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_ fluxk.f
-----						
3.7%	13.4	9.6	42.2%	1,411,772,930,846,618	22,424,492,033	line.36
1.1%	4.0	7.0	64.9%	369,435,907,219,731	6,575,931,964	line.54
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_ fluxi.f
-----						
1.1%	4.1	4.9	55.7%	452,998,790,837,684	6,904,792,416	line.807
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_ fluxj.f
-----						
2.8%	10.2	18.8	66.0%	1,077,521,395,774,529	16,750,162,451	line.36
8.2%	29.3	40.7	59.0%	3,118,214,977,991,204	48,910,720,877	line.76
=====						

COMPUTE | STORE | ANALYZE

# Code in FLUXK Responsible for Memory Bandwidth Utilization



```
73.      M m
74.    + M m ib-----<
75.    + M m ib i-----<
76.      M m ib i Vbr4--<>
77.      M m ib i          >
78.      M m ib i----->
79.      M m ib
80.      M m ib
81.      M m ib
82.      M m ib          >
83.      M m ib
84.      M m ib
85.      M m ib
86.      M m ib D-----<
87.      M m ib D
88.      M m ib D          >
89.      M m ib D----->
90.      M m ib
91.      M m ib
92.      M m ib----->
```

```
      DO K = 1, KCMAX
        DO L = 1, 5
          DQ(1:IND,J,K,L) = DQ(1:IND,J,K-1,L)
          DTV(1:IND,J,K) * (FSK(1:IND,K,L) - FSK(1:IND,K-1,L))
        ENDDO

      IF (ISGSK .EQ. 1) THEN
        DQ(1:IND,J,K,7) = DQ(1:IND,J,K,7) -
          DTV(1:IND,J,K) * (FSK(1:IND,K,7) - FSK(1:IND,K-1,7))
      ENDIF

      IF ( ICHM .GT. 0 ) THEN
        DO L = 8, 7 + NSPECI
          DQ(1:IND,J,K,L) = DQ(1:IND,J,K,L) -
            DTV(1:IND,J,K) * (FSK(1:IND,K,L) - FSK(1:IND,K-1,L))
        ENDDO
      ENDIF
    ENDDO
```





# Array Syntax and Automatic Blocking by the Compiler

# A



by 33% -  
ere 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) - FSK(I,K-1,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          ENDIFF
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          ENDIFF
93.      M m 3 V
94.      M m 3 V----->      ENDDO
95.      M m 3----->      ENDDO
96.      M m----->>      ENDDO
```

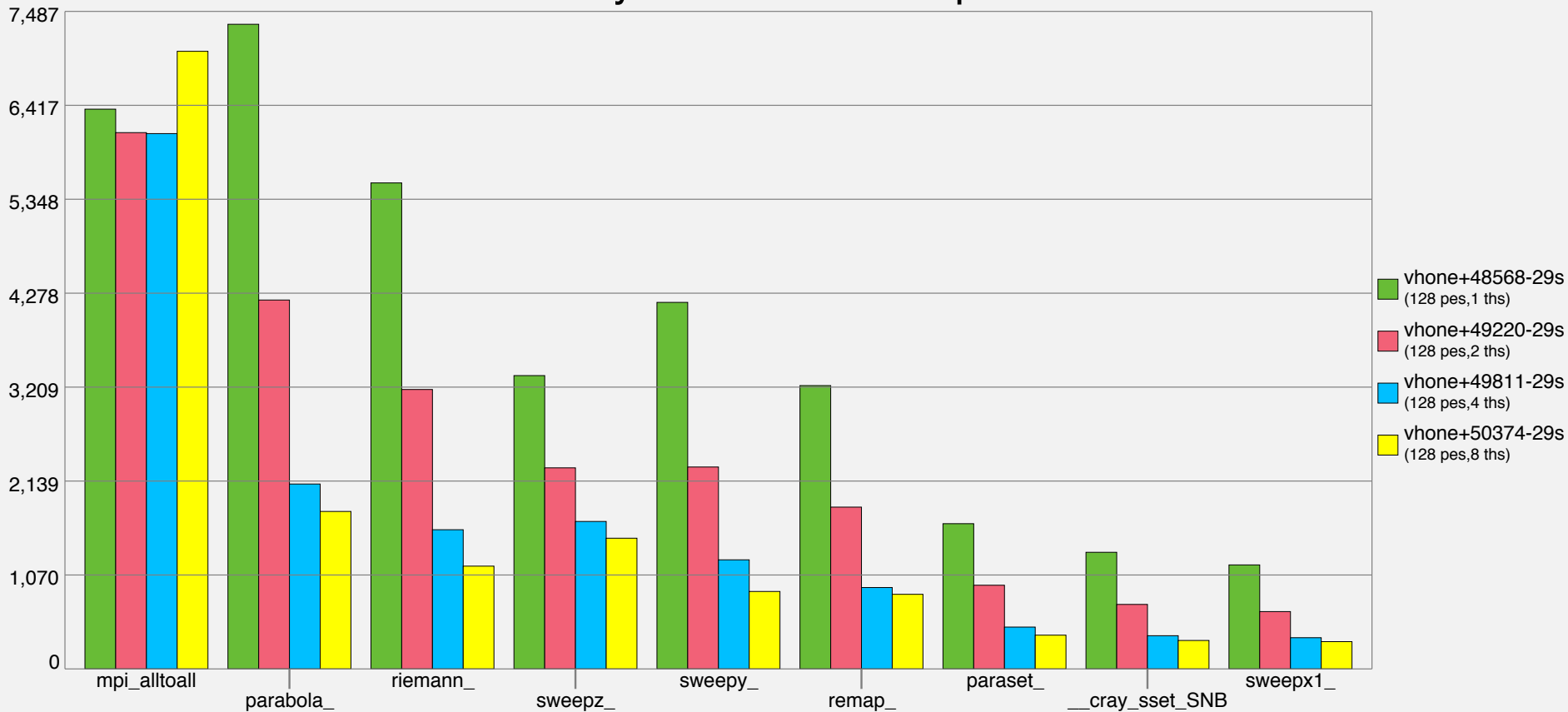
# Whacked

# VH1

# VH1 Already Parallelized Using Reveal

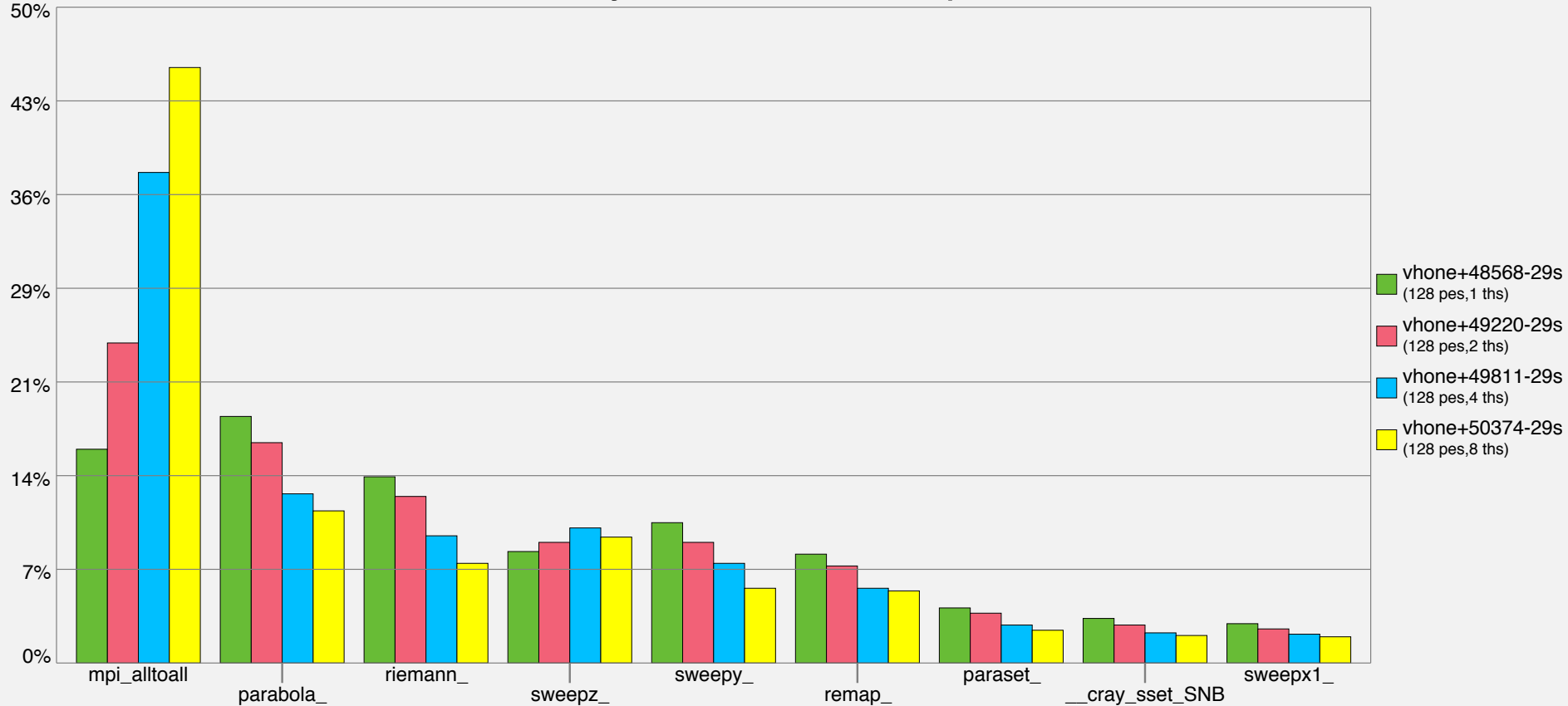
- **Need to investigate additional optimization**
- **Vectorization and Memory utilization optimization**

# Routines by Number of Samples



COMPUTE | STORE | ANALYZE

# Routines by Percent of Samples



COMPUTE | STORE | ANALYZE

# Profile for 1 Thread and 4 Threads

Table 1: Profile by Function 1 Thread

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

# Do Loop Table

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

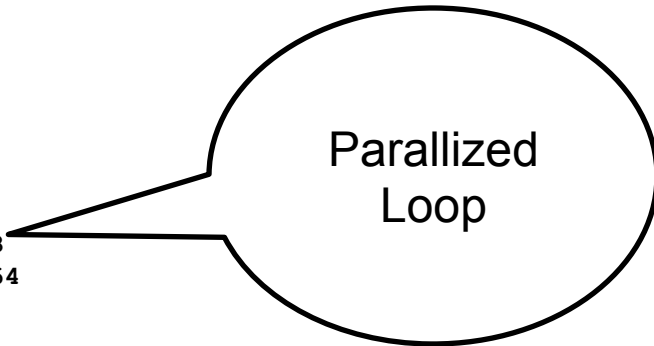
Loop Incl Time%	Loop Incl Time	Loop Hit	Loop Trips Avg	Loop Trips Min	Loop Trips Max	Function=/.LOOP[.] PE=HIDE
100.0%	631.108612	1	50.0	50	50	vhone_.LOOP.2.li.205
30.6%	193.127659	100	64.0	64	64	sweepy_.LOOP.1.li.38
30.6%	193.127263	6,400	128.0	128	128	sweepy_.LOOP.2.li.39
27.8%	175.704223	50	128.0	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	COMPL50.0   sweepz_(exclusive)



ANALYZE



# 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)*diffa(n) + para(n,2)*da(n+1) + para(n,3)*da(n)	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	.9%		31.3		14.7		32.0%		line.55
56.	fV	al(n) = flat(n) * a(n) + onemfl * al(n)	4	.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	.4%		13.6		10.4		43.5%		line.67
68.	f	deltaa(n) = ar(n) - al(n)	4	.8%		27.2		13.8		33.9%		line.68
69.	f	a6(n) = 6. * (a(n) - .5 * (al(n) + ar(n)))	4	.4%		15.4		11.6		43.2%		line.69
70.	f	scrch1(n) = (ar(n) - a(n)) * (a(n)-al(n))	4	.4%		13.4		10.6		44.3%		line.70
71.	f	scrch2(n) = deltaa(n) * deltaa(n)	4	.4%		14.0		12.0		46.2%		line.71
72.	f	scrch3(n) = deltaa(n) * a6(n)	4	0.1%		4.8		8.2		63.5%		line.72
73.	f----	enddo	4	0.3%		10.2		9.8		49.1%		line.73
74.			4	0.6%		19.4		14.6		43.1%		line.74
75.	Vr2--<	do n = nmin, nmax	4	0.5%		17.9		11.1		38.4%		line.75
76.	Vr2	if(scrch1(n) <= 0.0) then	4	1.2%		40.6		16.4		28.8%		line.80
77.	Vr2	ar(n) = a(n)	4	1.8%		63.9		24.1		27.5%		line.81
78.	Vr2	al(n) = a(n)	4	0.0%		0.2		2.8		92.7%		line.82
79.	Vr2	endif	4	0.1%		4.3		7.7		64.4%		line.84
80.	Vr2	if(scrch2(n) + <scrch3(n)) al(n) = 3. * a(n) - 2. * ar(n)	4	0.5%		16.0		12.0		43.2%		line.85
81.	Vr2	if(scrch2(n) < -scrch3(n)) ar(n) = 3. * a(n) - 2. * al(n)	4	0.6%		21.3		13.7		39.4%		line.86
82.	Vr2-->	enddo	4	0.0%		0.0		1.0		95.7%		line.87
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										

PARABOLA



COMPUTE

STORE

ANALYZE

# 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) - prghi(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) - prghi(l)))
74. 1 2 umidl(l) = ulft(l) - (pmid(l) - plft(l)) / wlft(l)
75. 1 2 umidr(l) = urgh(l) + (pmid(l) - prghi(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.



# 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    wfft(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    wfft(l) = clft(l) * sqrt(wfft(l))
69. 1 2    wrgh(l) = crgh(l) * sqrt(wrgh(l))
70. 1 2    zlft(l) = 4.0 * vlft(l) * wfft(l) * wfft(l)
71. 1 2    zrgh(l) = 4.0 * vrgh(l) * wrgh(l) * wrgh(l)
72. 1 2    zlft(l) = -zlft(l) * wfft(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)) / wfft(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    wfft(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    wfft(l) = clft(l) * sqrt(wfft(l))
70. 1 Vr2    wrgh(l) = crgh(l) * sqrt(wrgh(l))
71. 1 Vr2    zlft(l) = 4.0 * vlft(l) * wfft(l) * wfft(l)
72. 1 Vr2    zrgh(l) = 4.0 * vrgh(l) * wrgh(l) * wrgh(l)
73. 1 Vr2    zlft(l) = -zlft(l) * wfft(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)) / wfft(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    if (abs(pmid(l)-pmold(l))/pmid(l) < tol ) then
80. 1 Vr2    converged(l) = .T.
81. 1 Vr2    endif
82. 1 Vr2    endif
83. 1 Vr2    enddo
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
```

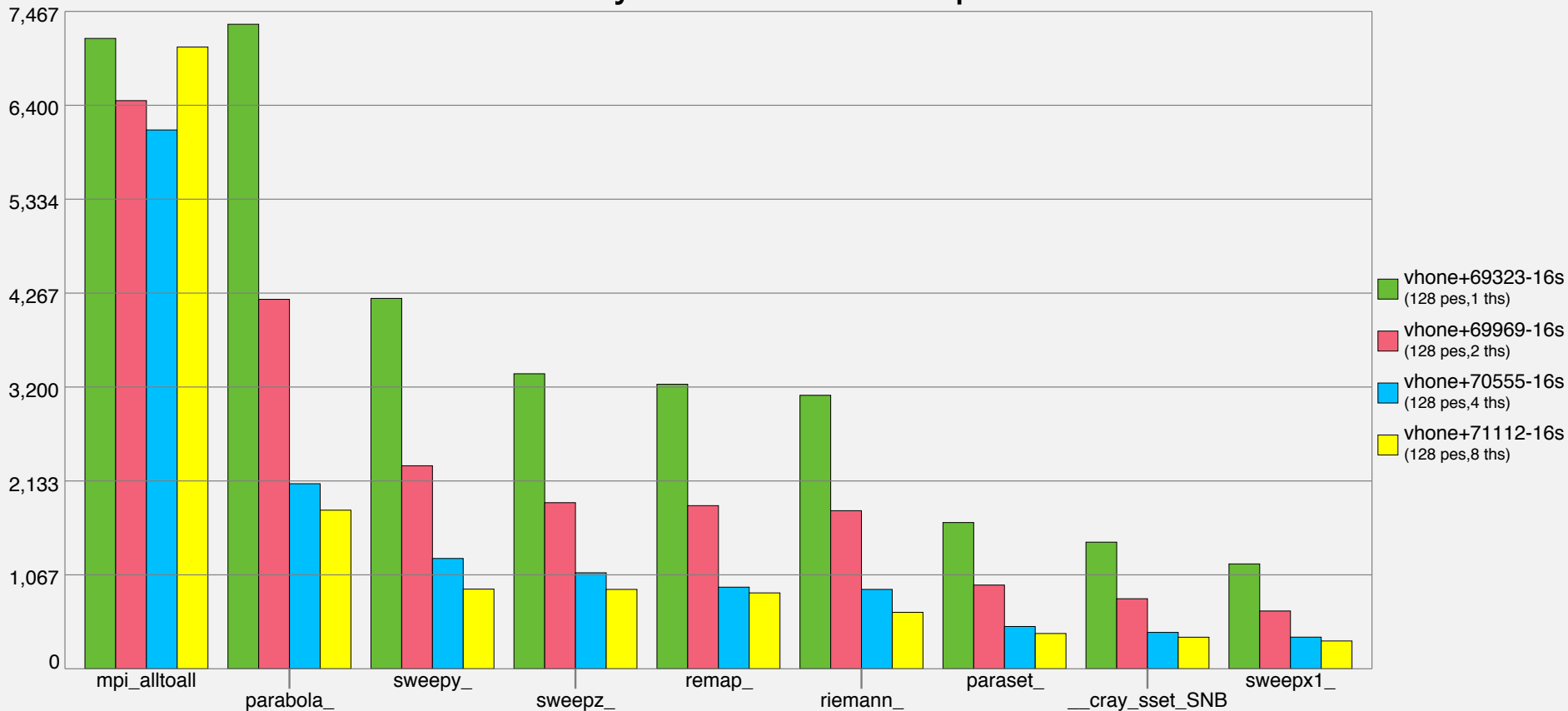
# SWEEPZ

```
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
```

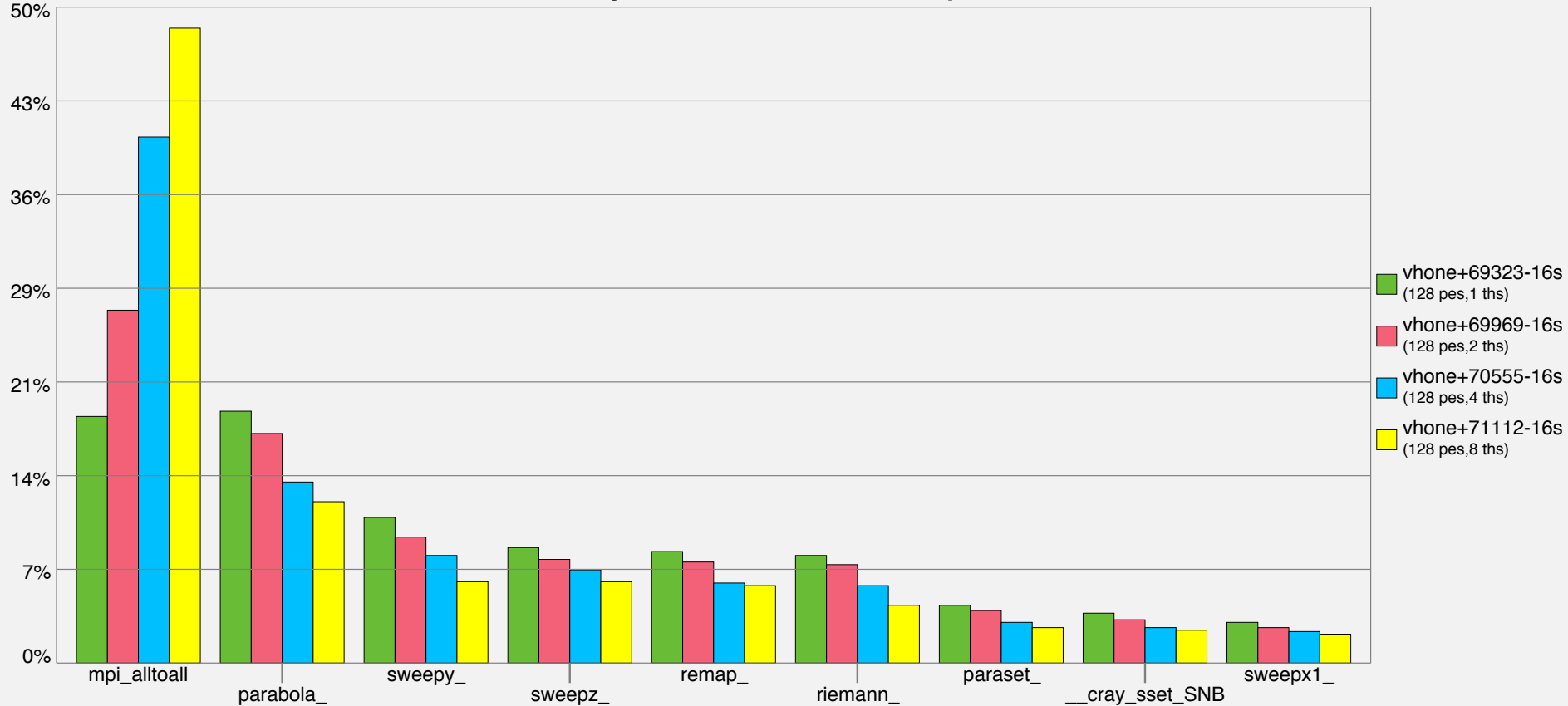
# Routines by Number of Samples



COMPUTE | STORE | ANALYZE



# Routines by Percent of Samples



COMPUTE | STORE | ANALYZE

# Profile for 1 Thread and 4 Threads

Table 1: Profile by Function 1 Thread

Samp%	Samp	Imb. Samp	Imb. Samp%	Group
				Function=[MAX10]
				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. Samp	Imb. Samp%	Group
				Function=[MAX10]
				PE=HIDE
				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. Samp	Imb. Samp%	MEM_LOAD_UOPS_RETIRED :HIT_LFB:precise=2	RESOURCE_STALLS :ANY	Group Function=[MAX10] Source Line 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_ parabola.f90
-----						
14.0%	71.1	77.9	52.7%	7,540,450,746,779,697	113,994,086,387	line.26
1.0%	5.2	8.8	63.0%	510,173,395,620,708	8,400,427,348	line.32
8.1%	41.0	41.0	50.4%	4,241,915,862,200,189	65,974,673,046	line.46
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_ sweepy.f90
-----						
3.2%	16.2	19.8	55.6%	1,653,665,489,088,910	27,467,001,609	line.46
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_ sweepz.f90
-----						
2.4%	12.3	19.7	62.0%	1,356,797,349,204,156	21,098,054,630	line.28
1.8%	8.9	13.1	60.0%	945,580,000,330,081	13,804,851,073	line.65
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  COMPUTE | STORE | ANALYZE
```

Difficult to merge these loops – compiler did merge two

# 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 waterfront, likely Copenhagen, featuring colorful buildings and a prominent church spire, reflected in the water. The sky is clear and blue.

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